

MODELLING OF ATMOSPHERIC CRUDE DISTILLATION COLUMN

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in Partial Fulfilment of the Requirements
for the Degree of

MASTER OF TECHNOLOGY

by

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CERTIFICATE

It is certified that the present work entitled,
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has been carried out by Mr. Ujjwal Manna under my supervision
and that it has not been submitted elsewhere for a degree.

May , 1986



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NOMENCLATURE

$A_{j,i}$	Absorption factor for ith component at jth stage
\overline{A}_i	Submatrices in the Jacobian
A_i	Elements in coefficient matrix of the component material balance equation
\overline{B}_i	Submatrices in the Jacobian
B_i	Elements in coefficient matrix of the component material balance equations
\overline{C}_i	Submatrices in the Jacobian
C_i	Elements in coefficient matrix of the component material balance equations
D	Distillate flow rate, kg mole/h
D_i	Right hand side of component material balance equation
E_j	Discrepancy function of enthalpy balance equation at jth stage
$E_{j,i}$	Murphree plate efficiency of ith component on jth plate
F_j	Total molar flow rate of feed at jth stage, kg mole/h
\overline{F}	Vector of functions
$f_{j,i}$	Component (ith) flow rate of feed at jth stage $\frac{\text{kg mole}}{\text{h}}$
G_i	Right hand side of component material balance equations for crude distillation problem
$H_{j,i}$	Enthalpy of ith component at jth stage in vapor phase
H_j	Stream enthalpy of vapor at jth stage, kcal/kg mole
H_j^{steam}	Enthalpy of steam being introduced at jth stage, kcal/h
H_F	Enthalpy of vapor portion of feed, kcal/h
$h_{j,i}$	Enthalpy of ith component at jth stage in liquid phase, kcal/kg mole
h_j	Stream enthalpy of liquid at jth stage, kcal/kg mole

h_F	Enthalpy of liquid portion of feed, kcal/kg mole
i	ith component
\bar{J}	Jacobian matrix
j	jth stage
$K_{j,i}$	K-value of ith component at jth stage
K	Watson characterization factor
k	Iteration number
L_j	Total liquid flow rate at jth stage, kgmole/h
$l_{j,i}$	Component (ith) liquid flow rate at jth stage, kgmole/h
M_j	Discrepancy function for overall material balance equation at jth stage
M	Number of components
N	Number of equilibrium stages
P	Operating pressure, psia
P_C	Critical pressure, psia
P_r	Reduced pressure
P^S	Vapor pressure, psia
P_{br}^S	Reduced vapor pressure
p	Elements of coefficient matrix of component material balance equations after forward substitution
Q_j	Heat removal at jth stage, kcal/h
Q_C	Condenser heat duty, kcal/h
Q_R	Reboiler heat duty, kcal/h
R	Reflux ratio
s_j	Fraction of vapor withdrawn from jth plate; Discrepancy function of summation equations at jth stage

s_j	Fraction of liquid withdrawn from jth plate
SG	Specific gravity, 60°F/60°F
T_j	Temperature of jth stage, °C
T_b	Normal boiling point, °R
T_c	Critical temperature, °R
T_r	Reduced temperature
T_{br}	Reduced boiling point
V_j	Total vapor flow rate at jth stage, kgmole/h
$v_{j,i}$	Component (ith) flow rate at jth stage, kgmol/h
V_r	Reduced volume
W_j	Liquid side stream drawn from jth plate, kgmol/h
W_j^*	Liquid side stream drawn for pumparound reflux at jth stage, kgmol/h
\bar{X}	Vector of independent variables
$\Delta \bar{X}$	Correction vector of variables
$x_{j,i}$	Molefraction of ith component at jth stage in liquid phase
$x_{F,i}$	Mole fraction of feed
$y_{j,i}$	Mole fraction of ith component at jth stage in vapor phase
$z_{j,i}$	Mole fraction ith component in feed at jth stage
Z	Compressibility factor

Greek Letters

β	Damping factor
ϵ	Tolerance limit
ω	Acentricity factor
ρ	Coefficient matrix of component material balance equations

Subscripts

i component number

j stage number

F refers to feed

Superscripts

k iteration number

ABSTRACT

A method, using simultaneous equation solving technique, has been developed to solve multicomponent distillation problems and then extended to simulate a crude-oil distillation column. The crude oil is assumed to be composed of a number of pseudo-components whose thermodynamic properties are correlated with their average boiling points and specific gravities. In this method, the equilibrium, overall material balance and enthalpy balance equations have been solved simultaneously with L , V , T as independent variables using Broyden's procedure. Component material balance equations were solved using modified Thomas algorithm as have been proposed by Hoefling and Seader. Fractionation problems having large number of components of wide volatility range can be solved by this method. Its convergence characteristics have been found to be satisfactory. The memory requirement is also low which is important for columns with large number of trays and feeds containing many components.

CHAPTER 1

INTRODUCTION

Petroleum industry is one of the biggest among the chemical industries with an annual throughput of about 40 million tonnes of crude oil. The entire crude oil to be processed by a petroleum refinery has to pass through the crude distillation unit or more commonly called topping unit which makes it the most important of all process equipment in refinery. Therefore the importance of rating or design of distillation columns processing crude oil or any other petroleum fractions is imaginable. Before the advent of modern fast computing machines, people used empirical methods and rules of thumb to design crude distillation columns. With the rapid growth of electronic computers, a number of methods of multicomponent distillation calculations have been published (Amundson and Pontinen, 1958, Sujata, 1961, Rose et al. 1958, Tomich, 1970, Naphthali and Sandholm, 1971 etc.). Consequently interest to simulate or design distillation columns processing petroleum fractions using computers has also grown. But till date very few papers have been published in this regard compared to the steady supply of papers on multicomponent distillation in Chemical Engineering journals. The refineries still continue to use empirical correlations and thumb rules for design of their distillation units. It is not the lack of interest in use of modern methods of computation on the

part of petroleum refiners which has prevented them from using these tools, rather, it is the lack of appropriate procedures which are applicable to their problems. Although crude distillation like most other distillation problems is a multicomponent, multistage process, yet it differs significantly from other conventional columns. Whereas, in conventional multicomponent distillation units, the feed consists of a specified number of identifiable chemical compounds to which thermodynamic properties can be assigned uniquely, it is neither practical nor possible to identify the constituents of a crude oil. Therefore special procedures are required to characterize the crude oil to enable the estimation of thermodynamic properties such as vapor-liquid equilibria, enthalpies etc. In addition to the above difficulties the complex nature of the tower configuration having side strippers, unconventional type of reflux, heat removal at intermediate plate create further computational problems. Wide boiling range of the petroleum fractions to be distilled from crude oil may lead to additional problems in convergence.

In the present study, attempt has been made to model a petroleum fractionator by considering the feed to be composed of a finite number of pseudo-components to which thermodynamic properties can be assigned on the basis of their average boiling point and density. Once the feed is characterized in

this fashion, any multicomponent calculation procedure could be used for rating of a refinery distillation column. In this study, a modified version of Tomich (1970) method has been used.

The whole thesis has been organised in the following way. The second chapter contains literature review of computational methods for multicomponent fractionation in general. The third chapter describes features and problems specific to crude oil distillation. The formulation of the model by the present method is included in chapter four. The fifth chapter contains the results of computation obtained by the present model and compares them with those obtained with a standard commercial package. The last chapter presents the conclusion drawn and recommendations for future work.

CHAPTER 2

LITERATURE REVIEW

In this chapter major developments in the field of simulation of multicomponent fractionation have been reviewed with an emphasis on Newton-Raphson technique used in solving these problems.

2.1 Simulation of Multicomponent Fractionation:

Since the advent of modern fast computers there have been many articles published in literature which use plate to plate rigorous calculation. This trend in multicomponent calculation started with the historic article by Thiele and Geddes (1933). This study used the sequential method of calculation where starting from both ends of the column plate by plate calculations were made sequentially until the feed plate was reached. The convergence in these type of plate to plate calculation methods was usually slow which was promoted by a modification introduced by Lyster et al. (1959) called the ' θ method' of convergence promotion. Pondon et al. (1973) proposed a multi- θ method where a different theta was used for each plate. The application of θ - method of convergence has been demonstrated by Holland (1981). Things turned in a different direction using more elegant mathematical techniques, when Amundson and Pontinen (1958) proposed a formulation in

which one writes the necessary material balance equations in a compact matrix form which can be solved by efficient algorithms such as the Thomas algorithm. A variation of this type of method was proposed by Sujata (1961) which is popularly known as the 'sum rate' or SR method, whereas the original one is termed as the 'Bubble point' or BP method. These two methods differ in their way of updating temperature in each iteration. The BP method utilises bubble point calculation and computes vapor flow rate from enthalpy balance equations, whereas the 'SR' method computes the total vapor flow rate by summing up the component flow rates which are obtained by solving tridiagonal coefficient matrix and then evaluates the temperature profile from enthalpy balance equations. The 'BP' method is generally applicable to close boiling mixtures, hence best suited for distillation problems, whereas the 'SR' method can solve wide boiling mixtures, like the kind faced in absorption problems. The applicability of these methods has been discussed by King (1971). Rose et al. (1958) introduced a different approach in multicomponent calculations popularly known as 'Relaxation technique'. It follows the transient behaviour of separation processes approaching steady state and uses a relaxation factor. The successful application of this method depends upon the choice of optimal value of this factor.

Tomich (1970) and Naphthali-Sandholm (1971) proposed two methods which used multivariate Newton-Raphson (NR) technique

in solving multicomponent problems. These two methods can be termed as simultaneous methods where material and energy balance equations along with the equilibrium relations are solved simultaneously. This is in contrast to the 'BP' and 'SR' methods which are successive iteration methods. The simultaneous methods are considered to be superior to successive ones since in the former, all the necessary variables in the functions are corrected simultaneously as distinguished from the latter class of methods where only one set is corrected at a time. These two methods need be described in greater detail as our present method owes its origin to these two methods. These have been presented in Sections 2.2 and 2.3. Ketchum (1975) proposed a new method which combines the salient features of both NR technique and Relaxation method. This method strives to attain the speed of convergence of NR method while retaining the stability of relaxation method. Hlavacek (1981) introduced one parameter imbedding technique in multicomponent calculation. Also different authors have tried to use NR method by grouping the variables and error functions in different ways. Notable among these is a paper by Ferraris et al. (1982) which is considered to be suitable for systems having one component of either very high or very low volatility. This method can be applicable to systems having steam present as one component such as steam strippers. This method can be considered as a variation of Naphthali-Sandholm technique. Chakraborty (1982)

has shown several different variants of Naphthali-Sandholm method.

2.2 Tomich's Method:

This procedure basically solves component material balance equations with a tridiagonal matrix algorithm. Heat balance and summation equations are handled with a quasi-Newton method. A notable feature of this method is that, in a mathematical sense, all equations are solved simultaneously.

2.2.1 Description of the Model Column:

The model column for mathematical simulation is shown in Figure 1. Because of the general form, the model represents all types of stage-by-stage separation processes, though in the figure a distillation column is shown. Feed streams can be introduced on each tray of the model. Vapor and liquid stream can also be withdrawn from each plate. Similarly heat can be added to or withdrawn from each tray to simulate reboilers, side heaters, interchillers and condensers.

2.2.2 Model Equations:

The basic equations for column simulation are derived by making material and heat balances around j th tray of the model (Figure 2). Heat and mass balances plus equilibrium relationships comprise five sets of equations to be solved.

(i) Overall material balance equations:

$$L_{j-1} - (1+s_j) L_j - (1+s_j) V_j + V_{j+1} + F_j = 0$$

$$N-1 \geq j \geq 2$$

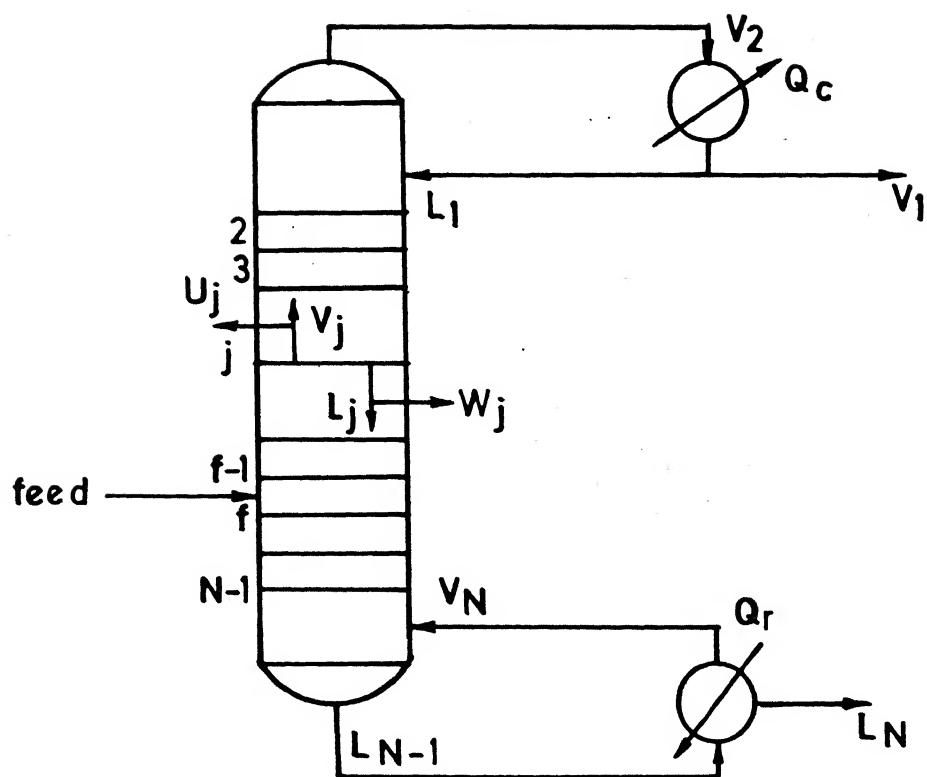


FIG.1 MODEL COLUMN

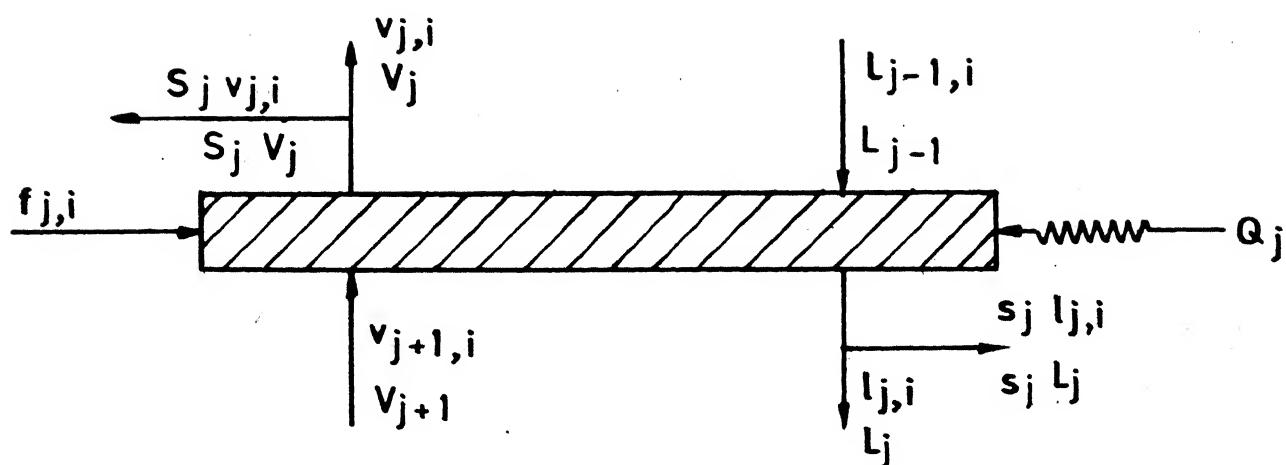


FIG. 2 MODEL TRAY

$$\begin{aligned}
 V_{j+1} - L_j - V_j &= 0 & ; & \quad j = 1 \\
 L_{j-1} - V_j - L_j &= 0 & ; & \quad j = N
 \end{aligned}
 \tag{2.1}$$

where L = liquid flow rate

V = vapor flow rate

s_j = fraction of liquid drawn off = $\frac{W_j}{L_j}$

S_j = fraction of vapor drawn off = $\frac{U_j}{V_j}$

F = feed rate

N = total number of plates

Subscript $j-1$, j , $j+1$ represent the $(j-1)$ th, j th and $(j+1)$ th plate respectively.

(ii) Vapor-liquid equilibrium relations:

$$\begin{aligned}
 y_{j,i} - K_{j,i} x_{j,i} &= 0 & ; & \quad 1 \leq i \leq M \\
 & & \text{and} & \quad 1 \leq j \leq N
 \end{aligned}
 \tag{2.2}$$

where K = distribution coefficient

y = mole fraction in vapor phase

x = mole fraction in liquid phase

M = number of components

Subscript i refers to the i th component.

(iii) Component material balance equations:

$$\begin{aligned}
 V_{j+1} y_{j+1,i} + L_{j-1} x_{j-1,i} + F_j z_{j,i} - (1+s_j)L_j x_{j,i} \\
 - (1+S_j)V_j y_{j,i} &= 0 & ; & \quad 1 \leq i \leq M \\
 & & \text{and} & \quad 2 \leq j \leq N-1
 \end{aligned}$$

$$\begin{aligned}
 V_{j+1} y_{j+1,i} - L_j x_{j,i} - V_j y_{j,i} &= 0 \quad ; \quad 1 \leq i \leq M \\
 &\text{and} \quad j = 1 \\
 L_{j-1} x_{j-1,i} - L_j x_{j,i} - V_j y_{j,i} &= 0 \quad ; \quad 1 \leq i \leq M \\
 &\text{and} \quad j = N
 \end{aligned}
 \tag{2.3}$$

where z = mole fraction in feed

(iv) Summation equations:

$$s_j = \sum_{i=1}^M y_{j,i} - \sum_{i=1}^M x_{j,i} = 0; \quad 1 \leq j \leq N
 \tag{2.4}$$

(v) Heat balance equations:

$$\begin{aligned}
 E_j &= [V_{j+1} H_{j+1} + L_{j-1} h_{j-1} + F_j h_j^F \\
 &\quad - (1+s_j)L_j h_j - (1+s_j)V_j H_j] - Q_j = 0 \\
 &\quad ; \quad 2 \leq j \leq N-1 \\
 E_j &= V_{j+1} H_{j+1} - L_j h_j - V_j H_j - Q_c = 0 \\
 &\quad ; \quad j = 1 \\
 E_j &= L_{j-1} h_{j-1} - L_j h_j - V_j H_j + Q_r = 0 \\
 &\quad j = N
 \end{aligned}
 \tag{2.5}$$

where h = liquid stream enthalpy

H = vapor stream enthalpy

h^F = feed stream enthalpy

Q = heat removal rate at intermediate plate

Q_c = condenser heat duty

Q_r = reboiler heat duty

2.2.3 Method of Solution:

Equation set (2.2) can be substituted into set (2.3) to eliminate $x_{j,i}$ and reduce the component material balance equations to the tridiagonal matrix form for the case of simple distillation columns.

$$\begin{bmatrix} B_1 & 1 & & & \\ C_2 & B_2 & 1 & & \\ & C_3 & B_3 & 1 & \\ & - & - & - & - \\ & & & C_{N-1} & B_{N-1} & 1 \\ & & & & C_N & B_N \end{bmatrix} \begin{bmatrix} v_{1,i} \\ v_{2,i} \\ v_{3,i} \\ - \\ v_{N-1,i} \\ v_{N,i} \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \\ D_3 \\ - \\ D_{N-1} \\ D_N \end{bmatrix}$$

$1 \leq i \leq M$
 (2.6)

In arriving at the above equations, use has been made of the fact that $v_{j,i} = V_j y_{j,i}$ and $l_{j,i} = L_j x_{j,i}$ where $v_{j,i}$ and $l_{j,i}$ are the vapor flow rate and liquid flow rate of i th component leaving j th stage respectively.

Also $B_1 = -(R+1)$ for total condenser,

where R is reflux ratio.

$$\begin{aligned}
 B_j &= - \left[(1+S_j) + (1+s_j) A_{j,i} \right] \\
 A_{j,i} &= L_j / (V_j K_{j,i}) \\
 C_j &= A_{j-1,i} \\
 D_j &= -F_j Z_{j,i}
 \end{aligned}$$

This set of equations (2.6) is a linear or nearly linear set when K-values are composition independent or weak-functions of composition. The procedure to solve all the equations is summarized stepwise as follows:

1. Initial values of T_j and V_j are assumed for all j .
2. L_j^i 's are computed from equation set (2.1).
3. Equation set (2.6) is solved using Thomas algorithm (Lapidus, 1962) or any other efficient algorithm to give $v_{j,i}$'s and hence $y_{j,i}$'s.
4. Equation set (2.2) is solved to give $x_{j,i}$'s.
5. These results are substituted in equation sets (2.4) and (2.5) which are solved simultaneously by Broyden's procedure to give a new set of T_j and V_j .
6. With these new values of T_j and V_j , calculations from step 2 through step 5 are repeated until convergence is achieved.

Convergence criterion used in this case is

$$\sum_{j=1}^N (E_j^2 + S_j^2) \leq \epsilon \quad (2.7)$$

where ϵ is preassigned tolerance limit.

2.2.4 Critique of Tomich's Method:

It is a general method which can be used for any type of multicomponent fractionation problem such as distillation,

absorption etc. By using simultaneous equation solving procedure, it eliminates numerical instability which occurs in sequential approach due to build-up of truncation errors. Use of quasi-Newton method reduces computation time. Since, for each iteration, Jacobian and its inverse need not be calculated. Tomich's method requires less memory space compared to other methods using NR technique like Naphthali-Sandholm's method because of less number of iterated variables. However, this method fail to converge for highly nonideal solutions.

2.3 Naphthali-Sandholm Method:

In this procedure, the equations of conservation of mass and energy and equilibrium relations are grouped together stagewise and then solved by linearizing them. The resulting set of equations has a block tri-diagonal structure.

Figure 2 represents a model plate whose side streams are specified by the ratio of the side stream to the stream which remains after they are withdrawn. In this formulation $l_{j,i}$, $v_{j,i}$, T_j are the independent variables whereas L_j , V_j representing the total phase flows within the column are dependent variables. The plates may have a feed stream introduced to it and there may be heat removal from or heat addition to it as before.

2.3.1 Model Equations:

(i) Enthalpy balance equations:

$$E_j = \sum_{i=1}^M \left[(1 + s_j) v_{j,i} H_{j,i} + (1 + s_j) l_{j,i} h_{j,i} - l_{j-1,i} h_{j-1,i} - v_{j+1,i} H_{j+1,i} - f_{j,i} h_{j,i}^F \right] + Q_j$$

; $1 \leq i \leq M$
and $2 \leq j \leq N-1$

(2.8)

where H = enthalpy of components in vapor phase

h = enthalpy of components in liquid phase

h^F = enthalpy of components in feed stream

f = component flow rate in feed stream

s_j = fraction of vapor withdrawn from j th plate

$$= U_j / V_j$$

s_j = fraction of liquid withdrawn from j th plate

$$= W_j / L_j$$

(ii) Component material balance equations:

$$M_{j,i} = (1 + s_j) v_{j,i} + (1 + s_j) l_{j,i} - v_{j+1,i} - l_{j-1,i} - f_{j,i}$$

; $1 \leq i \leq M$
and $2 \leq j \leq N-1$

(2.9)

(iii) Vapor-liquid equilibrium relations:

$$Q_{j,i} = \frac{E_{j,i} K_{j,i} V_j l_{j,i}}{L_j} - v_{j,i} + \frac{(1 - E_{j,i}) v_{j+1,i} V_j}{V_{j+1}}$$

; $1 \leq i \leq M$ & $2 \leq j \leq N-1$

(2.10)

where E = Murphree plate efficiency

$Q_{j,i}$ is derived from the definitions of the vapor phase murphree plate efficiency, that is

$$E_{j,i} = \frac{y_{j,i} - y_{j+1,i}}{K_{j,i} x_{j,i} - y_{j+1,i}} \quad (2.11)$$

or

$$E_{j,i} K_{j,i} x_{j,i} - y_{j,i} + (1 - E_{j,i}) y_{j+1,i} = 0 \quad (2.12)$$

where x and y represent mole fractions in liquid and vapor phase respectively. In terms of component flow rates it becomes

$$E_{j,i} K_{j,i} \frac{l_{j,i}}{L_j} - \frac{v_{j,i}}{V_j} + (1 - E_{j,i}) \frac{v_{j+1,i}}{V_{j+1}} = 0 \quad (2.13)$$

Multiplying both sides by V_j equation (2.10) is arrived.

2.3.2 Method of Solution:

These functions apply to all intermediate plates of the column. They can also be applied to partial condensers and reboilers provided reboiler heat duty and condenser heat duty are known. There can also be different other specifications possible which are detailed in the paper (Naphthali and Sandholm, 1971). There are $(2M+1)$ number of variables and same number of functions for each stage or a total of $N(2M+1)$ variable and equations. These are grouped stagewise. In compact form these can be written as

$$\bar{F}(\bar{X}) = 0 \quad (2.14)$$

where $\bar{X} = [\bar{X}_1, \bar{X}_2, \bar{X}_3, \dots, \bar{X}_N]^T$

$\bar{F} = [\bar{F}_1, \bar{F}_2, \bar{F}_3, \dots, \bar{F}_N]^T$

$\bar{X}_j = [v_{j,1}, v_{j,2}, \dots, v_{j,M}, T_j, l_{j,1}, l_{j,2}, \dots, l_{j,M}]^T$

$\bar{F}_j = [E_j, M_{j,1}, M_{j,2}, \dots, M_{j,M}, Q_{j,1}, Q_{j,2}, \dots, Q_{j,M}]^T$

Thus using this notation the NR method becomes,

$$\bar{X}^{m+1} = \bar{X}^m + \Delta \bar{X}^{m+1} \quad (2.15)$$

where $\Delta \bar{X}^{m+1} = -\bar{J}^{-1} \bar{F}^m \quad (2.16)$

$\Delta \bar{X}^{m+1}$ is the correction added to \bar{X}^m to get the new values of the variables \bar{X}^{m+1} . Here superscript m and $m+1$ refer to iteration number. If the functions are linear, this correction would make the value of each function equal to zero. Since the functions are nonlinear, $\Delta \bar{X}^{m+1}$ is just an approximation to the needed correction. \bar{J} is the Jacobian matrix that is the matrix of partial derivatives of all the functions with respect to all of the variables at present value of the variable \bar{X}^m . Hence

$$\bar{J} = \left(\frac{\partial \bar{F}}{\partial \bar{X}} \right) = \begin{bmatrix} \frac{\partial \bar{F}_1}{\partial X_1} & \frac{\partial \bar{F}_1}{\partial X_2} & \dots & \frac{\partial \bar{F}_1}{\partial X_N} \\ \frac{\partial \bar{F}_2}{\partial X_1} & \frac{\partial \bar{F}_2}{\partial X_2} & \dots & \frac{\partial \bar{F}_2}{\partial X_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial \bar{F}_N}{\partial X_1} & \frac{\partial \bar{F}_N}{\partial X_2} & \dots & \frac{\partial \bar{F}_N}{\partial X_N} \end{bmatrix} \quad (2.17)$$

where

$$\frac{\partial^2 F_i}{\partial X_j} = \begin{bmatrix} \frac{\partial F_{i,1}}{\partial X_{j,1}} & \frac{\partial F_{i,1}}{\partial X_{j,2}} & \dots & \frac{\partial F_{i,1}}{\partial X_{j,2M+1}} \\ \frac{\partial F_{i,2}}{\partial X_{j,1}} & \dots & \dots & \frac{\partial F_{i,2}}{\partial X_{j,2M+1}} \\ \vdots & & & \\ \frac{\partial F_{i,2M+1}}{\partial X_{j,1}} & \dots & \dots & \frac{\partial F_{i,2M+1}}{\partial X_{j,2M+1}} \end{bmatrix} \quad (2.18)$$

It is noted that the functions for plate j involve only variables of $j-1$, j and $j+1$. Thus the partial derivatives of the functions on j th plate with respect to the variables on all plates other than these three are zero. So the Jacobian matrix takes the structure of a block tridiagonal form

$$J = \begin{bmatrix} \bar{B}_1 & \bar{C}_1 & & & \\ \bar{A}_2 & \bar{B}_2 & \bar{C}_2 & & \\ & & & \bar{A}_j & \bar{B}_j & \bar{C}_j \\ & & & & & & \bar{A}_{N-1} & \bar{B}_{N-1} & \bar{C}_{N-1} \\ & & & & & & & \bar{A}_N & \bar{B}_N \end{bmatrix} \quad (2.19)$$

where \bar{A} , \bar{B} , \bar{C} are individually matrices of the order $(2M+1)$.

$$\bar{A}_j = \left(\frac{\partial F_i}{\partial X_{j-1}} \right); \quad \bar{B}_j = \left(\frac{\partial F_i}{\partial X_j} \right); \quad \bar{C}_j = \left(\frac{\partial F_i}{\partial X_{j+1}} \right)$$

Detailed structure of these sub-matrices can be found in the original paper referred above.

Newton Raphson method by itself is often unstable, specially when the initial guesses are far from the solution. To reduce the chances of divergence, a damping method may be used in which,

$$\bar{X}^{m+1} = \bar{X}^m + \beta \Delta \bar{X}^{m+1} \quad (2.20)$$

The value of the damping parameter, β , should be chosen in such a way that $\sum \bar{F}^{m+1}$ is minimized. For this, any one dimensional-search technique like Golden Section method can be used. Even with β -modification it is important that initial guess is not far from the solution. One procedure to generate a reasonable initial guess is to assume a constant molal overflow and a linear temperature profile. Then, with composition independent K-values, solving the component material balance equations, component liquid and vapor flow rates through the column can be generated.

2.3.3 Critique of Naphthali-Sandholm Method:

This is a very general method which can be applied to any type of multicomponent calculations without having to modify it. Volatility range does not affect the method either. Without requiring any modifications, highly non-ideal solutions can also be treated because the presence of non-ideality is accounted for rigorously. Various types of specifications

can be taken into account in a rigorous manner through the equilibrium relations. Feeds can be added to or side streams can be withdrawn from any plate. Also heat can be added to or can be removed from any plate. The method is based on a linearization of distillation equations. So convergence accelerates as the solution is approached. No computational difficulties or complications arise from component flow being small. The primary disadvantage of this method is the huge amount of storage required. The size of the Jacobian matrix in this method is $N(2M+1) \times N(2M+1)$. Though with efficient memory saving algorithm like block Thomas algorithm only \bar{C}_j sub matrices need to be stored, with interconnected columns, the storage requirement goes up.

2.4 Interconnected Column:

The simulation of interlinked columns can be done by the same algorithm treating all the columns present as a single column. However, the ^{usual} statement "Functions of a plate contains only the variables of that plate and the two adjacent plates" - does not hold good any more due to the interconnections. Because of this, the Jacobian matrix contains some off-diagonal elements besides the tridiagonal band affecting the sparsity of the matrix. Stadtherr (1979) proposed a technique to maintain sparsity in process design calculations. Hidalgo et al. (1980) proposed an optimal arrangement of simultaneous linearized

equations for general systems of interlinked multistaged separators. They developed an algorithm which automatically arranges the linearized equations so that for a Newton-Raphson type of solution procedure (for example, Naphthali-Sandholm technique), a minimum or nearly minimum number of non-zero blocks occur outside the tridiagonal band. In this way, computational memory and time requirements are minimized.

Hoeffling and Seader (1978) proposed an algorithm to solve the tridiagonal matrix having offdiagonal elements, which is a modification of original Thomas algorithm. Seader et al. (1980) proposed an optimal arrangement of equations for interlinked columns to minimize the non-zero elements. Stadtherr et al. (1982) looked into various solution techniques for sparse matrices, common in multistage separators. Stadtherr (1982) in another paper proposed an algorithm which rearranged the block tridiagonal matrix having off-diagonal elements into bordered block tridiagonal form and then applied block triangular splitting technique to solve it. This algorithm is comparable to Hoeffling-Seader's algorithm in efficiency.

CHAPTER 3

CRUDE OIL DISTILLATION

Crude oil distillation is one type of distillation which still needs special attention, inspite of many general purpose package available commercially because of complexity of crude composition, unconventional type of column configuration and its operation. In this chapter the process of crude oil distillation will be described briefly and then the major methods available for its calculation will be discussed.

3.1 Distillation Column:

Unlike the mixtures treated in usual distillation columns which are made up of a few discrete components, crude oil consists of a very large number of hydrocarbons all the way from methane to materials having 70 or more carbon atoms, the exact composition of which is nearly impossible to determine. Therefore the way to characterize crude oil or a petroleum fraction for the purpose of its fractionation is to determine the boiling point curves from results obtained in laboratory test distillation units. Depending upon the operating conditions there can be different types of boiling curves like TBP, ASTM, EFV. The specifications and operating conditions of the apparatus to obtain these curves are given in detail by Nelson (1958). True Boiling Point or TBP distillation is usually

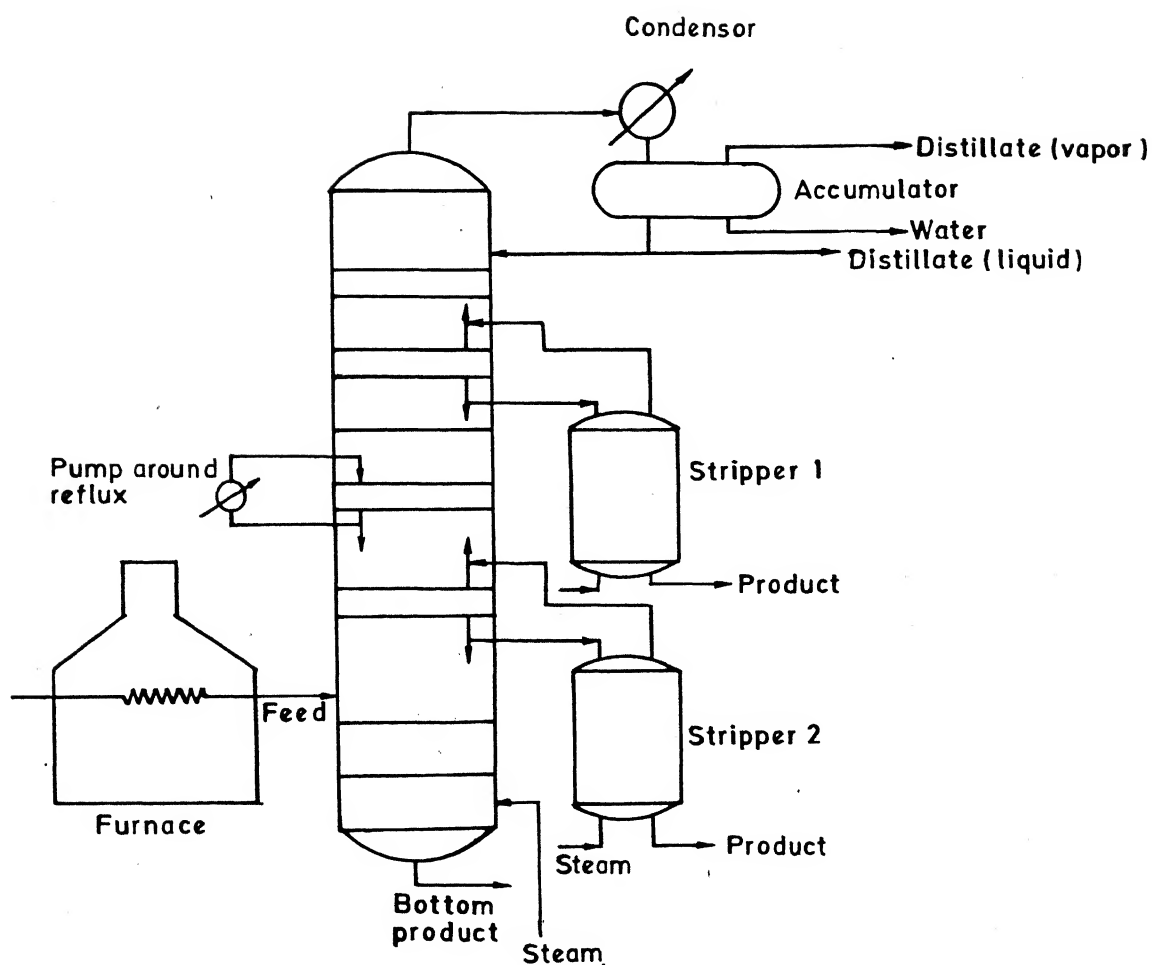


FIG. 3 A TYPICAL ATMOSPHERIC CRUDE DISTILLATION TOWER

run on crude oil and is indicative of its composition, whereas ASTM is run on different petroleum fractions and used by designers to specify a certain fraction. EFV distillation is seldom run due to its high cost. All other properties are assigned to the fractions by correlating these properties with the average boiling point and density of the fractions.

In crude-oil distillation, the crude is preheated in a furnace and then flashed in the flash-zone of the distillation tower. A schematic diagram of a typical refinery crude distillation unit is shown in Figure 3. A small amount of extra vaporization, called overflash, is employed to provide adequate reflux between the flash zone i.e. the point at which partially vaporized feed is introduced and lowest side stream product draw tray. All the heat supplied to the column comes through the preheated feed, as there is no reboiler in the tower. Open steam is introduced into the column to strip the lighter components from the bottom product as well as to bring down the operating pressure effectively. Liquid products are withdrawn from different points of the column through side streams. Lighter components are stripped by open steam from these side-streams in side-strippers and then sent back to the column. Apart from top tray reflux, heat removal at intermediate points is attained by withdrawing an internal liquid stream from the tower, cooling it and then returning it to the column. The lightest distillate is not always condensable at the conditions

of temperature and pressure in the reflux drum and thus may be treated as two distillate fractions, one vapor and the other liquid.

3.2 Methods of Calculation:

There are two major trends in crude-oil distillation calculation. The first one is empirical in nature and is based upon Packin's method (1941) and second one utilizes the pseudo-component concept. We briefly discuss these methods below.

3.2.1 Empirical Methods:

In this method, for petroleum fractions, two terms are used to describe product composition and the degree of separation between two adjacent streams. ASTM boiling range defines the general composition of the fraction and is usually one of the key specifications for most distillates. The second term (5-95) gap signifies the relative degree of separation between adjacent streams. It is defined as the difference between 5 volume percent ASTM temperature of the heavy fraction and 95 volume percent ASTM temperature of the adjacent light fractions.

$$(5-95) \text{ gap} = (t_{5_H} - t_{95_L}) \text{ ASTM, degrees Fahrenheit} \quad (3.1)$$

In this method, the degree of difficulty of separation is defined as the difference between the 50 volume percent temperatures of the fractions under consideration. The 'separation

capability' of the system is defined as the product of the reflux to feed ratio at the upper draw tray (as calculated on a volumetric basis) and the number of trays in that section. The product is designated as F-factor. In the systems where pump-around reflux is used for heat removal the trays employed in this service are regarded as one-third of an actual fractionating tray. The degree of separation attainable and the (5-95) gap are defined as functions of the separation capability of the system (i.e. F-factor) with parameters of degree of difficulty of separation (i.e. Δt_{50} ASTM). The functions or correlations are basically empirical in nature. Later Packie's method has been extended by Watkins (1969).

3.2.2 Pseudo-Component Methods:

In this method, the crude mixture is considered to be composed of a number of pseudo-components or fractions, each of which having been assigned average properties such as boiling point, molecular weight, density, critical and other properties. The basic steps in this method are briefly stated below.

From the TBP-curve of the crude oil feed (see Figure 4) a number of constant temperature cuts are stepped off so that areas above and below the line between it and TBP-curve are equal (for example area abc = area cde in Figure 4). These cuts are termed as pseudo-components. The present components are considered to have average boiling points equal to those constant temperatures. For step abcde (Figure 4) the pseudo-

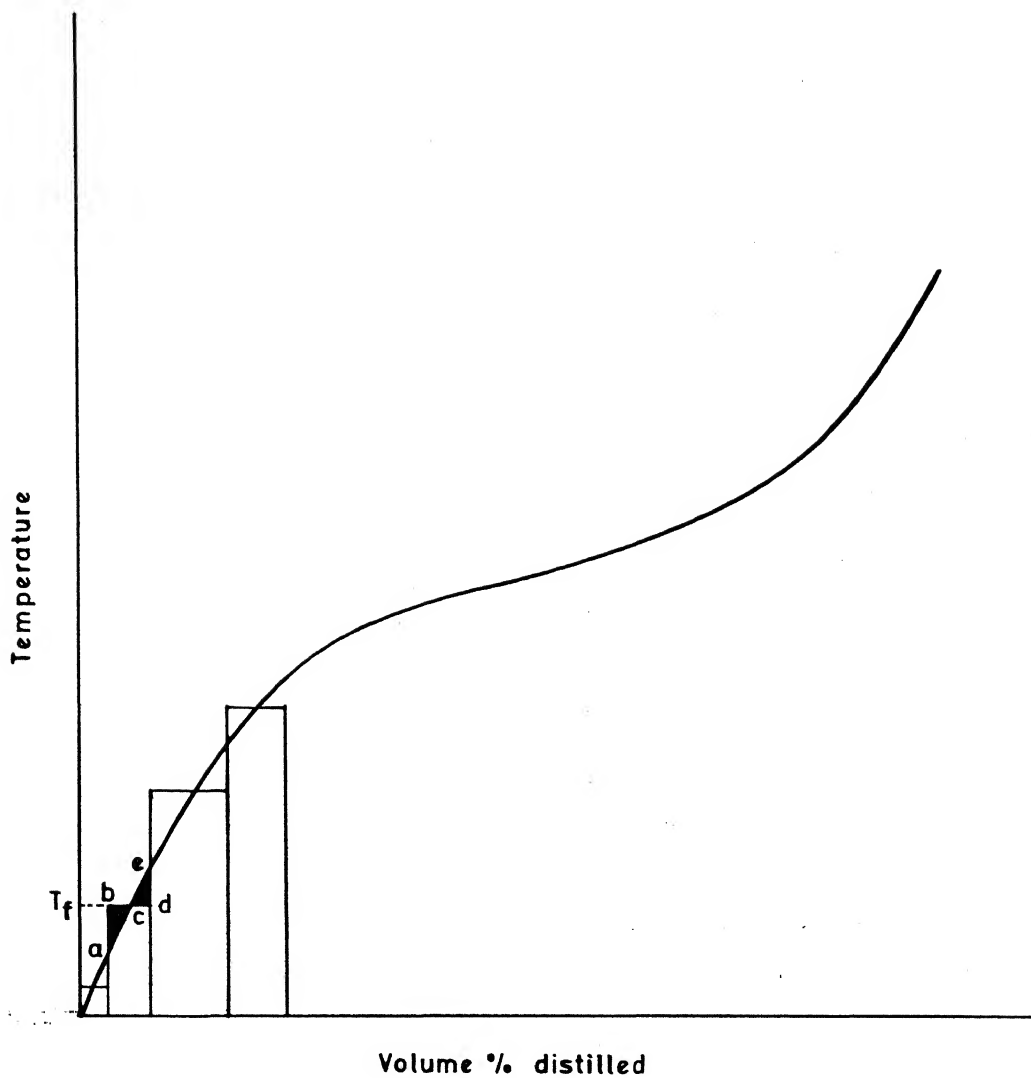


FIG. 4 BREAKUP OF TBP CURVE OF CRUDE OIL INTO PSEUDO COMPONENTS

component has the boiling point T_f . The number of these cuts is decided upon the preciseness of the separation desired. The width of these steps need not be equal. In the regions where the TBP-curve is sharp, the step width can be small whereas in flatter regions of the curve steps can be wider i.e. number of pseudo-components can be fewer. The density-midpercent curve is drawn from the experimental data on the cuts and hence each cut is assigned an average value of density. The molecular weight, watson characterization factor, critical parameters, acentricity factors of the cuts or the pseudo-components are determined from various correlation involving the boiling point and density.

To get the mole fractions of each-component in the feed mixture, the volume of each cut is converted to weight. The weight of each cut is then divided by its molecular weight to get the moles of each cut and they are summed up to give total molar flow of the feed. Then individual moles of each component is divided by total number of moles in the feed to give its mole fraction in the feed. Thus having got the mole fractions of the pseudo-components in the feed and having assigned molecular properties to each pseudo-component, any short cut method of multicomponent calculation or any rigorous technique as described in Chapter 2 can be applied for simulation of crude oil distillation. Prater and Boyd (1955) used this pseudo-component concept along with short cut methods

to design crude oil distillation tower. Cecchetti et al. (1963) first solved a crude oil distillation problem using this pseudo-component concept and a rigorous technique of multi-component distillation. They used Thiele-Geddes calculational procedure with θ - method of convergence. They split the crude oil into 34 pseudo-components. In their treatment an analogue of the actual column was found by trial. Analogue of the actual column is defined as a column having such number of theoretical plates that gives the same product stream as obtained from the actual column. Later, Hess et al. (1978) solved the same problem using "2N Newton Raphson technique". The difference in their approach was that whereas Cecchetti et al. assumed water vapor to be present only in the vapor phase throughout the column, Hess et al. considered water to be present in both phases.

3.2.3 Other Methods:

Besides above two approaches, a few others have tried somewhat different methods to solve crude distillation problems. Notable among these is the work of Nikolaj (1970) who solved crude oil distillation problem by making different modules for different sections of the column. These modules can be solved independently. Material and energy balance calculations were done around each module. The properties of the product streams of the modules were computed by using empirical correlations.

By making different combinations of these modules, different problems having different tower configurations can be solved.

3.3 A Critique on Crude Oil Distillation Calculations:

It should be emphasized that no method, including the pseudo-component method, is exact because of the assumptions necessary to assign average properties to each of the pseudo-components. In principle, the pseudo component method will approach exactness as the number of cuts approaches infinity. It is, however, not practical to make more than about 50 pseudo-component which may not provide a reasonable approximation to the actual feed. To assign thermodynamic properties to these components, one uses generalized correlations which may introduce further uncertainties in calculations, since it is very difficult to accurately correlate these properties with the available specifications. Precise vapor-liquid equilibrium data are very difficult if not impossible to obtain. It is nearly impossible to define and thus evaluate stage efficiencies. This problem can be tackled in a round about way by defining an analogue column for a particular distillation unit. However, once an analogue of a particular column is found by trial and error it can be used to solve any problem with that column.

CHAPTER 4

MODELLING OF CRUDE OIL DISTILLATION

Naphthali-Sandholm is by far the best method available for multicomponent calculations. But its use is limited because of its large memory requirement. The Jacobian matrix in this type of formulation is of the order of $N(2M+1)$ and for systems having a large number of components it can create a great deal of problem. For simple distillation problems where there are no interconnections present, the Jacobian matrix will have a regular shape of block tri-diagonal form because of stage-wise grouping of variables. Different efficient memory saving algorithms can take care of this type of problem without much difficulty. But with interconnections present, as in case of a column with side strippers, elements also appear in positions other than the tri-diagonal band in the Jacobian matrix resulting in its greater fill-in. In crude oil distillation due to intermediate refluxes, the structure of the blocks also get changed. For these reasons, Naphthali-Sandholm method can not be applied very easily to solve this type of problem.

Another alternative is Tomich's method which has low memory requirements. Its Jacobian matrix is of the order of $2N$ but without the tridiagonal band structure. As mentioned

earlier (Section 2.2.4), its convergence characteristics can be poor. Chakraborty (1983) has reported the use of some variants of Naphthali-Sandholm method which have better convergence characteristics than Tomich's method, though poorer in convergence with respect to the original Naphthali-Sandholm method. In the present work, we have chosen the functions similar to those suggested by Chakraborty. The dependent variables, however, no longer depend only on adjacent stages which leads to the loss of block tridiagonal matrix characteristic of Naphthali-Sandholm method and its variants. The present formulation deviates from that of Tomich in the sense that while Tomich assumed and corrected temperature and total vapor flow rate on each stage simultaneously and subsequently calculated liquid flow rates, in the present case, all the three variables T_j , V_j and L_j are assumed and corrected simultaneously.

Although in the present study, the formulation as discussed above has been used, advantages of Naphthali-Sandholm method cannot be discounted. The non-availability of enough storage in computer prevented the testing of Naphthali-Sandholm method for crude-oil distillation problem in the present study. But the formulation has been included in Appendix A and it is hoped that this approach will be tested at a later date.

4.1 Modelling of a Distillation Column Without Interconnections:

Before attempting to model crude oil distillation unit, the present approach has been applied to a conventional multicomponent distillation column without interconnections. Since such columns can as easily be simulated by Naphthali-Sandholm or other methods, this exercise enables us to establish the validity of this approach to at least such problems.

4.1.1 The Model:

The model plate of figure (2) is considered once again. The equations describing the plate were presented as equations 2.1 through 2.5. Substituting the value of $l_{j,i}/L_j$ from equation (2.2) into equation (2.4), the following equation is obtained:

$$\frac{1}{V_j} \sum_{i=1}^M \left(\frac{1}{K_{j,i}} - 1 \right) v_{j,i} = 0 \quad ; \quad j = 1, 2, \dots, N \quad (4.1)$$

Following three functions are chosen for iterative calculations.

The equilibrium relations:

$$s_j = \frac{1}{V_j} \sum_{i=1}^M \left(\frac{1}{K_{j,i}} - 1 \right) v_{j,i} \quad ; \quad j = 1, 2, \dots, N \quad (4.2)$$

For partial condenser and partial reboiler the equilibrium relations remain unchanged.

The overall material balance equations:

$$M_j = L_{j-1} - (1 + s_j) L_j - (1 + S_j) V_j + V_{j+1} + F_j \quad ; \quad j = 2, 3, \dots, N-1$$

$$\begin{aligned}
 M_j &= V_{j+1} - L_j - V_j & ; \quad j = 1 \\
 M_j &= L_{j-1} - L_j - V_j & ; \quad j = N
 \end{aligned} \tag{4.3}$$

The enthalpy balance equations:

$$E_j = \sum_{i=1}^M (l_{j-1,i} h_{j-1,i} - (1+s_j) l_{j,i} h_{j,i} - (1+S_j) v_{j,i} H_{j,i} + v_{j+1,i} H_{j+1,i} + f_{j,i} h_{j,i}^F) ; \quad j = 2, 3, \dots, N-1$$

The enthalpy balance equations for $j=1$ are replaced by the following specification equations.

$$E_1 = L_1 - RV_1$$

$$\text{or} \quad E_1 = V_1 - D$$

where R = reflux ratio

D = distillate flow rate

For the reboiler ($j=N$) specification equations become,

$$E_N = T_N - T_N^*$$

$$\text{or} \quad E_N = L_N - L_N^* \tag{4.4}$$

where T_N^* and L_N^* are the specified temperature of and liquid draw off from the reboiler respectively. There can be other specifications also possible, like, reboiler heat duty or reboil ratio. For total condenser, the equilibrium equation is replaced by a specification equation. The specification in this case may be condenser temperature or condenser heat duty.

4.1.2 Method of Solution:

For the three functions (Equations 4.2, 4.3 and 4.4) at each plate, the chosen independent or iterated variables are

T_j , L_j and V_j . In function form these equations become,

$$\bar{F}(\bar{X}) = 0$$

where $\bar{F} = [\bar{F}_1, \bar{F}_2, \dots, \bar{F}_N]^T$

$$\bar{F}_j = [S_j, M_j, E_j]^T$$

and $\bar{X} = [\bar{X}_1, \bar{X}_2, \dots, \bar{X}_N]^T$

$$\bar{X}_j = [T_j, L_j, V_j]^T$$

For a given set of values of the independent variables, the dependent variables $v_{j,i}$ and $l_{j,i}$ can be found in the following way. The vapor phase component flow rate $v_{j,i}$ can be computed by solving equation (2.6), $l_{j,i}$ can then be calculated using following relations

$$l_{j,i} = A_{j,i} v_{j,i} \quad (4.5)$$

where $A_{j,i} = L_j/V_j K_{j,i}$

There are three equations at each plate, namely, equations 4.2, 4.3 and 4.4 and also there are three unknowns, namely, T_j , L_j and V_j for which those equations are to be solved. For a total of N plates, therefore, there is a set of $3N$ equations in as many variables to be solved simultaneously. The major steps involved in the solution are as follows:

Step 1: Assume initial values of T_j , L_j and V_j 's which form the group vector \bar{X}^0 .

Step 2: With these values of T_j , L_j and V_j 's solve equations (2.6) and (4.5) to generate component flow rates

throughout the column. Thomas algorithm is used to solve equation set (2.6), since, the coefficient matrix has the tridiagonal band structure.

Step 3: Equations (4.2), (4.3) and (4.4) can now be solved using Broyden's algorithm which is discussed next.

Broyden's Method:

Broyden's method is based on the numerical approximation of the partial derivatives appearing in the Jacobian matrix (Broyden, 1965). This approach permits the inverse of the Jacobian matrix to be updated after each trial. Thus it is necessary to compute partial derivatives in the Jacobian matrix only once. As approximate values for the partial derivatives are used, it requires more iterations to converge to the solution. However, since it avoids computation of partial derivatives and its inversion with every iteration, it saves a lot of computer time per iteration, specially when numerical differentiation is used for the calculation of Jacobian matrix. In this method, the following calculations are performed to solve the set $\bar{F}(\bar{X}) = 0$.

S_j , M_j and E_j which are the elements of \bar{F}_j are really the errors or residuals in the equilibrium relation, material and heat balance equations and are equal to zero only when the solution is reached. These functions are expanded in Taylor series and terms containing derivatives of higher than first order are dropped to get

$$\bar{J} \Delta \bar{X} = -\bar{F} \quad (4.6)$$

where $\bar{J} = \begin{bmatrix} \frac{\partial \bar{F}_1}{\partial x_1} & \frac{\partial \bar{F}_1}{\partial x_2} & \dots & \frac{\partial \bar{F}_1}{\partial x_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial \bar{F}_N}{\partial x_1} & \frac{\partial \bar{F}_N}{\partial x_2} & \dots & \frac{\partial \bar{F}_N}{\partial x_N} \end{bmatrix}$

The structure of Jacobian is not of block-tridiagonal form as in the case of Naphthali-Sandholm method because the dependent variables $v_{j,i}$ and $l_{j,i}$ involved in equilibrium relations and enthalpy balance equations are dependent on temperature and total liquid and vapor flow rates of all the stages. The corrected values of the variables are

$$\bar{X}^{k+1} = \bar{X}^k + \beta^k \Delta \bar{X}^k \quad (4.7)$$

where k and $k+1$ are iteration numbers and β is a damping parameter and $\Delta \bar{X}^k$ is obtained from equation (4.6).

The following step by step procedure is employed to get the solution

Step 1: For assumed values of \bar{X}^0 , calculate

$$\bar{F}^0 = \bar{F}(\bar{X}^0)$$

Step 2: Define inverse of the Jacobian, as matrix \bar{H} which is updated in each iteration. As a first approximation, the elements of \bar{H}^0 are taken as,

$$\bar{H}^0 = - (\bar{J}^0)^{-1}$$

\bar{J}_0 is the matrix of the partial derivatives at the initial values of the variables. The partial derivatives are computed numerically as

$$\frac{\partial \bar{F}_i}{\partial \bar{X}_j} = \frac{\bar{F}_i(\bar{X}_i + \bar{h}_j) - \bar{F}_i(\bar{X}_j)}{\bar{h}_j}$$

where \bar{h}_j is a small increment which in the present case has been taken to be 0.1.

Step 3: From the values of \bar{H}^0 computed in step 2 and \bar{F}^0 computed in step 1, the correction vector $\Delta \bar{X}^0$ is calculated as

$$\Delta \bar{X}^0 = \bar{H}^0 \bar{F}^0$$

Step 4: A value of β^k ($k = 0, 1, 2, \dots$) is found such that the Euclidean norm of

$\bar{F}(\bar{X}^k + \beta^k \Delta \bar{X}^k)$ is less than that of $\bar{F}(\bar{X}^k)$ i.e.

$$\sum_i^n F_i^2(\bar{X}^k + \beta^k \Delta \bar{X}^k) < \sum_i^n F_i^2(\bar{X}^k)$$

where n is the total number of equations.

Finding the value of β^k is an iterative process in itself and can be started with an initial value of 1.0 i.e. $\beta_1^k = 1.0$

where subscript 1 is the iteration number for finding the optimum β^k for the K th iteration. For the calculation of

$\beta_2^K, \beta_3^K, \dots$ etc. the following relations are used.

$$\beta_{p+1}^k = \left[(1 + 6\eta)^{\frac{1}{2}} - 1 \right] / 3\eta$$

$$\eta = \frac{\sum_{i=1}^n F_i^2 (\bar{X}^k + \beta_P^k \Delta \bar{X}^k)}{\sum_{i=1}^n F_i^2 (\bar{X}^k)}$$

This procedure is continued until the norm is reduced. If after a specified number of iterations, the norm is not reduced, fresh partial derivatives are calculated at this point, as indicated in step 2.

Step 5: The next set of values for \bar{X} is computed as follows:

$$\bar{X}^{k+1} = \bar{X}^k + \beta^k \Delta \bar{X}^k \quad k = 0, 1, 2, \dots$$

The functions are evaluated with these new values of the variables and convergence is checked. If convergence criterion is not satisfied then \bar{H} is updated by the use of the following formulae:

$$\bar{F}^{k+1} = \bar{F}(\bar{X}^{k+1})$$

$$\bar{Y}^k = \bar{F}^{k+1} - \bar{F}^k$$

$$\bar{H}^{k+1} = \bar{H}^k - \frac{(\bar{H}^k \bar{Y}^k + \beta^k \Delta \bar{X}^k) \Delta \bar{X}^{kT} \bar{H}^k}{\Delta \bar{X}^{kT} \bar{H}^k \bar{Y}^k}$$

The convergence criterion used in this case is

$$\sum_{i=1}^n F_i^2(\bar{X}) \leq \epsilon$$

where ϵ is a preassigned tolerance limit.

Step 6: The new set of correction of variables is computed by following relation:

$$\Delta \bar{X}^{k+1} = \bar{H}^{k+1} \bar{F}(\bar{X}^{k+1}),$$

and the whole process is iterated from Step 2 until convergence is achieved.

4.1.3 An Example

A problem of operating distillation column processing mixture of eleven components has been solved using the model developed in previous subsection. This problem has been taken from Holland (1981) where solution by Thiele-Geddes method with θ - convergence is presented. (Table 1)

As seen in Table 2, the results obtained using present method compare well with those reported by Holland, thus establishing the validity of present method for solving multi-component distillation problem.

4.2 Modelling of Crude Oil Distillation Column:

In the previous section a model for a simple distillation column was considered. In this section, a model of a crude oil distillation column is described. The distillation column with three side strippers, two pump arounds and a total condenser is shown in Figure 5. Unlike the simple distillation column, in a crude oil distillation column there are different types of plates.

TABLE 1: STATEMENT OF THE PROBLEM

Component	FX_i	Specifications
CH_4	2.0	Reflux ratio = 2.0; boiling point liquid feed; partial condenser; column pressure = 300 psia; no. of stages = 12 and feed plate location = 5; reboiler temperature = 826°R. Equilibrium and enthalpy data for all components taken from Holland. (1981)
C_2H_6	10.0	
C_3H_6	6.0	
C_3H_8	12.5	
i- C_4H_{10}	3.5	
n- C_4H_{10}	15.0	
n- C_5H_{12}	15.2	
n- C_6H_{14}	11.3	
n- C_7H_{16}	9.0	
n- C_8H_{18}	8.5	
400 ⁺	7.0	

⁺Commonly referred to as 400°F - normal boiling fraction.

TABLE 2: COMPARISON OF RESULTS OBTAINED IN THE PRESENT
STUDY WITH THOSE OF HOLLAND

Component	Distillate composition in lb moles/hr calculated by		Bottom product composition in lb moles/hr calculated by	
	Present method	Holland (1981)	Present Method	Holland (1981)
CH ₄	0.2000 x 10	0.2000 x 10	0.6080 x 10 ⁻⁹	0.1116 x 10 ⁻⁸
C ₂ H ₆	0.9999 x 10	0.9999 x 10	0.7737 x 10 ⁻⁴	0.1162 x 10 ⁻³
C ₃ H ₈	0.5978 x 10	0.5972 x 10	0.2160 x 10 ⁻¹	0.2766 x 10 ⁻¹
C ₃ H ₈	0.1237 x 10 ²	0.1234 x 10 ²	0.1442	0.1535
i-C ₄ H ₁₀	0.7222	0.7421	0.2777 x 10	0.2757 x 10
n-C ₄ H ₁₀	0.4910	0.5360	0.1452 x 10 ²	0.1446 x 10 ²
n-C ₅ H ₁₂	0.1619 x 10 ⁻²	0.2015 x 10 ⁻²	0.1519 x 10 ²	0.1519 x 10 ²
n-C ₆ H ₁₄	0.7328 x 10 ⁻⁵	0.9403 x 10 ⁻⁵	0.1129 x 10 ²	0.1129 x 10 ²
n-C ₇ H ₁₆	0.4748 x 10 ⁻⁵	0.9402 x 10 ⁻⁵	0.9000 x 10	0.8999 x 10
n-C ₈ H ₁₈	0.3189 x 10 ⁻⁴	0.6342 x 10 ⁻⁷	0.8500 x 10	0.8499 x 10
400	0.4972 x 10 ⁻¹²	0.65162 x 10 ⁻⁷	0.7000 x 10	0.6999 x 10
Total	31.577	31.599	68.42	68.401

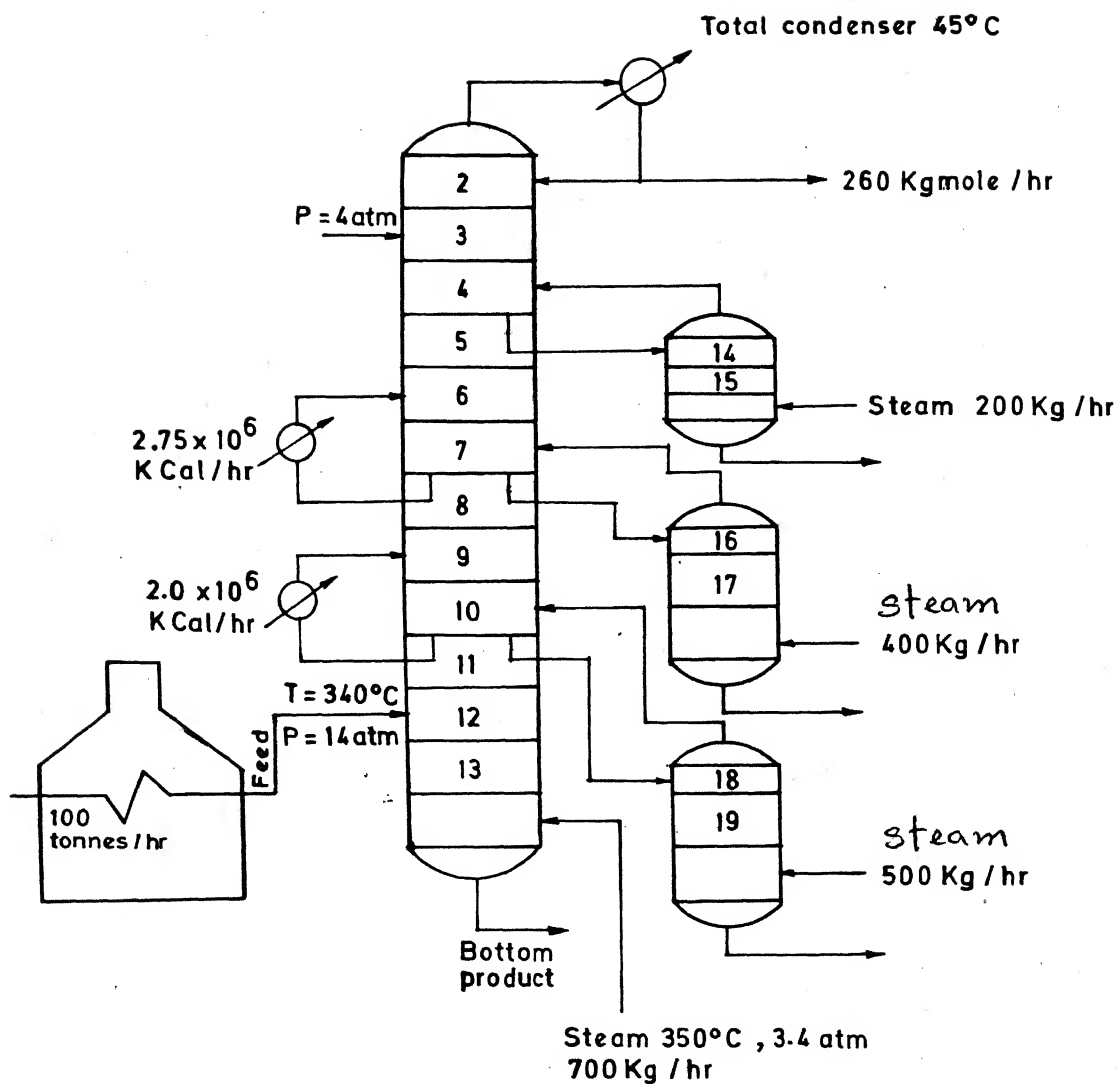


FIG.5 CRUDE OIL DISTILLATION TOWER SIMULATED IN THE PRESENT WORK

- (i) Plate representing condenser.
- (ii) Simple plate having no side stream and no pump around reflux.
- (iii) Plates from which liquid side stream is withdrawn
- (iv) Plates having pumparound reflux stream returned to them.
- (v) Plates where stripped out lighter components from the side-strippers are returned.
- (vi) Last plates of the column/side stripper where there is no vapor input from the plate below.
- (vii) First plates of the side strippers where feed is the liquid side stream draw-off from the main column.

Besides these differences, there is also a component (usually steam) in the system which is assumed to be present only in vapor phase and is designated as (M+1)th component.

4.2.1 The Model:

Each of the above types of plates will have different discrepancy functions for material and energy balance equations. In this subsection, all the equations describing the plates of a crude distillation column are presented.

Equilibrium Relations:

Combining equations (2.2) and (2.4) and taking into account of the fact that there is no water present in the liquid phase (i.e. $l_{j, M+1} = 0$, $j = 2, \dots, N$) the equilibrium discrepancy becomes,

$$S_j = \frac{1}{V_j} \left[\left(\sum_{i=1}^M \left(\frac{1}{K_{j,i}} - 1 \right) v_{j,i} \right) - v_{j,M+1} \right]$$

$$j = 2, \dots, N$$

If the condenser used is a total one the equilibrium discrepancy for first plate ($j=1$) is replaced by a specification equation,

$$S_1 = L_1 - RV_1 \quad (4.8)$$

$$\text{or} \quad S_1 = V_1 - D$$

Overall material balance equations:

For type (i) plate

$$M_j = V_{j+1} - L_j - V_j = 0 \quad ; \quad j = 1$$

For type (ii) plates

$$M_j = L_{j-1} - L_j - V_j + V_{j+1} + F_j = 0 \quad ; \quad j = 2, 5, 8, 11, 12$$

For type (iv) and (v) plates

$$M_j = L_{j-1} - L_j - V_j + V_{j+1} + V_m + W_{j+1}^i = 0 \quad ; \quad j=3, 6, 9$$

where subscript m refers to the number of sidestripper plate from which vapor is returned to the main column and W_{j+1}^i is the pumparound reflux stream.

For type (iii) plates

$$M_j = L_{j-1} - L_j - V_j - W_j - W_j^i + V_{j+1} = 0 \quad ; \quad j = 4, 7, 10$$

where W_j is the liquid side stream withdrawn for j th plate.

For type (vi) plates

$$M_j = L_{j-1} - L_j - V_j + f_j^{\text{steam}} = 0 \quad ; \quad j = 13, 15, 17, 19$$

where f_j^{steam} is the steam input to the column at j th stage.

For type (vii) plates

$$M_j = W_p - L_j - V_j + V_{j+1} = 0 \quad ; \quad j = 14, 16, 18 \quad (4.9)$$

where subscript p refers to the plate from which liquid side stream is withdrawn to be fed to the sidestrippers.

Component material balance equations:

$$v_{j+1,i} - l_{j,i} - v_{j,i} = 0 \quad ; \quad i = 1, \dots, M$$

and $j = 1$

$$l_{j-1,i} - l_{j,i} - v_{j,i} + v_{j+1,i} + f_{j,i} = 0 \quad ; \quad i = 1, \dots, M$$

and $j = 2, 5, 8, 11, 12$

$$l_{j-1,i} - \left(1 + \frac{W_j + W_j^s}{L_j}\right) l_{j,i} - v_{j,i} + v_{j+1,i} = 0 \quad ; \quad i = 1, \dots, M$$

and $j = 4, 7, 10$

$$l_{j-1,i} - l_{j,i} - v_{j,i} + v_{j+1,i} + \left(\frac{W_{j+1}^s}{L_{j+1}}\right) l_{j+1,i} + v_{m,i} = 0$$

; $i = 1, \dots, M$

and $j = 3, 6, 9$

$$\left(\frac{W_p}{L_p}\right) l_{p,i} - l_{j,i} - v_{j,i} + v_{j+1,i} = 0 \quad ; \quad i = 1, \dots, M$$

and $j = 14, 16, 18$

$$l_{j-1,i} - l_{j,i} - v_{j,i} = 0 \quad ; \quad i = 1, \dots, M$$

and $j = 13, 15, 17, 19$

(4.10)

Enthalpy balance equations:

$$E_j = \sum_{i=1}^M (l_{j-1,i} h_{j-1,i} - l_{j,i} h_{j,i} - v_{j,i} H_{j,i} + v_{j+1,i} H_{j+1,i} + f_{j,i} h_{j,i}^F) - v_{j,M+1} H_{j,M+1} + v_{j+1,M+1} H_{j+1,M+1} = 0$$

; $j = 2, 5, 8, 11, 12$

$$E_j = \sum_{i=1}^M (l_{j-1,i} h_{j-1,i} - l_{j,i} h_{j,i} - v_{j,i} H_{j,i} + v_{j+1,i} H_{j+1,i} \\ + (\frac{W_{j+1}^r}{L_{j+1}}) l_{j+1,i} h_{j+1,i} + v_{m,i} H_{m,i}) - v_{j,M+1} H_{j,M+1} \\ + v_{j+1,M+1} H_{j+1,M+1} + v_{m,M+1} H_{m,M+1} - Q_j = 0 \\ ; j = 3, 6, 9$$

where Q_j is the heat removal in pumparound stream at j th plate.

$$E_j = \sum_{i=1}^M (l_{j-1,i} h_{j-1,i} - v_{j,i} H_{j,i} - (1 + \frac{W_j + W_j^r}{L_j}) l_{j,i} h_{j,i} \\ + v_{j+1,i} H_{j+1,i}) - v_{j,M+1} H_{j,M+1} + v_{j+1,M+1} H_{j+1,M+1} = 0 \\ ; j = 4, 7, 10$$

$$E_j = \sum_{i=1}^N ((\frac{W_p}{L_p}) l_{p,i} h_{p,i} - l_{j,i} h_{j,i} - v_{j,i} H_{j,i} \\ + v_{j+1,i} H_{j+1,i}) - v_{j,M+1} H_{j,M+1} + v_{j+1,M+1} H_{j+1,M+1} = 0 \\ ; j = 14, 16, 18$$

$$E_j = \sum_{i=1}^M (l_{j-1,i} h_{j-1,i} - l_{j,i} h_{j,i} - v_{j,i} H_{j,i}) \\ - v_{j,M+1} H_{j,M+1} + f_j^{\text{steam}} H_j^{\text{steam}} ; j = 13, 15, 17, 19$$

where H_j^{steam} is the enthalpy of the steam being introduced into the j th plate.

For a total condenser ($j=1$) the enthalpy balance equation is replaced by one specification equation such as,

$$E_1 = T_1 - T_1^* = 0$$

where T_1^* is the specified condenser temperature.

There can be other types of specifications also possible such as condenser heat duty.

4.2.2 Method of Solution:

The chosen equations (4.8, 4.9, 4.11) are solved simultaneously using T_j , L_j and V_j as independent variables in the same way as for simple distillation discussed earlier in Section 4.1.2. The three major steps in the solution procedure discussed in that section are still valid except that in step 2, the Thomas algorithm needs to be modified since the coefficient matrix structure in component material balance equations is no longer tridiagonal. The following procedure based on modification due to Hoeffling and Seader (1978) can be substituted for that step. Substituting the expression for $l_{j,i}$ from equation (4.5) in equation set (4.10) the following relation is obtained.

$$\bar{\rho} \bar{v}_i = \bar{G}_i \quad (4.12)$$

where

$$\bar{v}_i = [v_{1,i} \ v_{2,i} \ \dots \ v_{N,i}]^T$$

$$\bar{G}_i = [0 \quad 0 \quad -f_{11,i} \ -f_{12,i} \ 0 \ \dots 0]^T$$

The structure of $\bar{\rho}$ matrix is shown in Table 3. A_i , B_i , C_i , are the elements of the tridiagonal band as usual and $A_{i,j}$ and $C_{i,j}$ are the off-diagonal elements in this coefficient matrix. As shown in this table, due to the presence of

TABLE 4: COEFFICIENT MATRIX AFTER FORWARD SUBSTITUTION (\bar{p}')

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
1	1	P_1																	
2		1	P_2																
3			1	P_3															
4				1	P_4														
5					1	P_5													
6						1	P_6												
7							1	P_7											
8								1	P_8										
9									1	P_9									
10										1	P_{10}								
11											1	P_{11}							
12												1	P_{12}						
13													1	P_{13}					
14														1	P_{14}				
15															1	P_{15}			
16																1	P_{16}		
17																	1	P_{17}	
18																		1	P_{18}
19																			1

interconnections in the column, there are six off-diagonal elements present in the matrix other than the tridiagonal band for this problem. The equation set (4.12) is solved using Hoeffling-Seader (1978) method of modified Thomas algorithm in which elements are forward substituted to give a matrix having only upper triangular elements. After forward substitution, equation (4.12) becomes

$$\bar{p}'_i \bar{v}_i = \bar{q}_i \quad (4.13)$$

where \bar{p}' is shown in Table 4. As seen from this table, because of the presence of off-diagonal elements, fill-ins occur in three discrete band. In this matrix main diagonal elements are all unity. p'_i 's are the elements in on-diagonal positions and the three off-diagonal bands are represented by the elements $p_{i,j}$'s. The elements of \bar{p} and \bar{q}_i will be obtained through the procedure described below:

Hoeffling-Seader Algorithm:

row 1: $p_1 \leftarrow C_1/B_1$; $q_1 \leftarrow G_1/B_1$
 row 2: $B_i \leftarrow (B_i - A_i p_{i-1})$
 $p_i \leftarrow C_i/B_i$; $q_i \leftarrow (G_i - A_i q_{i-1})/B_i$
 row 3: Same as row 2
 Add $p_{3,14} \leftarrow C_{3,14}/B_3$
 row 4-5: Same as row 2
 Add $p_{i,14} \leftarrow -A_i p_{i-1,14}/B_i$

row 6: Same as rows 4-5.

$$\text{Add } P_{6,16} \leftarrow C_{6,16}/B_6$$

row 7-8: Same as rows 4-5

$$\text{Add } P_{i,16} \leftarrow -A_i P_{i-1,16}/B_i$$

row 9: Same as rows 7-8.

$$\text{Add } P_{9,18} \leftarrow C_{9,18}/B_9$$

rows 10-12: Same as rows 7-8

$$\text{Add } P_{i,18} \leftarrow -A_i P_{i-1,18}/B_i$$

rows 13: $P_i \leftarrow -A_i P_{i-1,14}/B_i$

$P_{i,16}, P_{i,18}, q_i$ same as rows 10-12

row 14:

$$A_{14,i+1} \leftarrow -A_{14,i} P_i \quad ; \quad i = 4, \dots, 12$$

$$B_{14} \leftarrow (B_{14} - A_{14,i} P_{i,14}) \quad ; \quad i = 4, \dots, 12$$

Set $D_{14} \leftarrow -A_{14,6} P_{6,16}$

$$D_{14} \leftarrow (D_{14} - A_{14,i} P_{i,16}) \quad ; \quad i = 7, \dots, 13$$

Set $E_{14} \leftarrow -A_{14,9} P_{9,18}$

$$E_{14} \leftarrow (E_{14} - A_{14,i} P_{i,18}) \quad ; \quad i = 10, \dots, 13$$

Set $G_{14} \leftarrow G_{14}$

$$q_{14} \leftarrow (q_{14} - A_{14,i} q_i) \quad ; \quad i = 4, \dots, 13$$

$$B_{14} \leftarrow (B_{14} - A_{14,13} P_{13})$$

$$P_{14} \leftarrow C_{14}/B_{14}$$

$$P_{14,16} \leftarrow D_{14}/B_{14}$$

$$P_{14,18} \leftarrow E_{14}/B_{14}$$

$$q_{14} \leftarrow q_{14}/B_{14}$$

row 15:

$$B_i \leftarrow (B_i - A_i P_{i-1})$$

$$P_i \leftarrow -A_i P_{i-1,16}/B_i$$

$$P_{i,18} \leftarrow -A_i P_{i-1,18}/B_i$$

$$q_i \leftarrow (G_i - A_i q_{i-1})/B_i$$

row 16

$$A_{16,i+1} \leftarrow -A_{16,i} P_i \quad i = 7, \dots, 12$$

$$\text{Set } D_{16,14} \leftarrow -A_{16,7} P_{7,14} \quad i = 8, \dots, 12$$

$$A_{16,14} \leftarrow D_{16} - A_{16,13} P_{13}$$

$$A_{16,i+1} \leftarrow -A_{16,i} P_i \quad i = 14$$

$$B_{16} \leftarrow (B_{16} - A_{16,i} P_{i,16}) \quad i = 7, \dots, 14$$

$$B_{16} \leftarrow (B_{16} - A_{16,15} P_{15})$$

$$\text{Set } E_{16} \leftarrow -A_{16,9} P_{9,18}$$

$$E_{16} \leftarrow (E_{16} - A_{16,i} P_{i,18}) \quad i = 10, \dots, 15$$

$$\text{Set } q_{16} \leftarrow G_{16}$$

$$q_{16} \leftarrow q_{16} - A_{16,i} q_i \quad i = 7, \dots, 15$$

$$P_{16} \leftarrow C_{16}/B_{16}$$

$$P_{16,18} \leftarrow E_{16}/B_{16}$$

$$q_{16} \leftarrow q_{16}/B_{16}$$

row 17:

$$B_i \leftarrow (B_i - A_i P_{i-1})$$

$$P_i \leftarrow -A_i P_{i-1,18}/B_i$$

$$q_i \leftarrow (G_i - A_i q_{i-1})/B_i$$

row 18:

$$A_{18,i+1} \leftarrow -A_{18,i} P_i \quad i = 10, \dots, 12$$

$$\text{Set } D_{18} \leftarrow -A_{18,10} P_{10,14}$$

$$D_{18} \leftarrow D_{18} - A_{18,i} P_{i,14} \quad i = 11, 12$$

$$A_{18,14} \leftarrow (D_{18} - A_{18,13} P_{13})$$

$$A_{18,i+1} \leftarrow -A_{18,i} P_i \quad i = 14$$

Set $E_{18} \leftarrow -A_{18,10} P_{10,16}$

$$E_{18} \leftarrow E_{18} - A_{18,i} P_{i,16} \quad i = 11, \dots, 14$$

$$A_{18,16} \leftarrow (E_{18} - A_{18,15} P_{15})$$

$$A_{18,i+1} \leftarrow A_{18,i} P_i \quad i = 16$$

$$B_{18} \leftarrow (B_{18} - A_{18,i} P_{i,18}) \quad i = 10, \dots, 16$$

$$B_{18} \leftarrow (B_{18} - A_{18,17} P_{17})$$

$$P_{18} \leftarrow q_{18}/B_{18}$$

Set $q_{18} \leftarrow G_{18}$

$$q_{18} \leftarrow q_{18} - A_{18,i} q_i \quad i = 10, \dots, 17$$

$$q_{18} \leftarrow q_{18}/B_{18}$$

row 19: $B_i \leftarrow (B_i - A_i P_{i-1})$

$$q_i \leftarrow (G_i - A_i q_{i-1})/B_i$$

Following the above algorithm, after forward substitution, the matrix contains elements in upper triangle only. Applying backward substitution, then variables are solved as follows:

$$v_{19} \leftarrow q_{19}$$

$$v_i \leftarrow q_i - P_i v_{i+1} \quad i = 18, 17$$

$$v_i \leftarrow q_i - P_i v_{i+1} - P_{i,18} v_{18} \quad i = 16, 15$$

$$v_i \leftarrow q_i - P_i v_{i+1} - P_{i,18} v_{18} - P_{i,16} v_{16} \quad i = 14, 13$$

$$v_i \leftarrow q_i - P_i v_{i+1} - P_{i,18} v_{18} - P_{i,16} v_{16} - P_{i,14} v_{14} \quad i = 12, \dots, 9$$

$$v_i \leftarrow q_i - P_i v_{i+1} - P_{i,16} v_{16} - P_{i,14} v_{14} \quad i = 8, \dots, 6$$

$$v_i \leftarrow q_i - P_i v_{i+1} - P_{i,14} v_{14} \quad i = 5, \dots, 3$$

$$v_i \leftarrow q_i - P_i v_{i+1} \quad i = 2, 1$$

After having solved the component flow rates, Broyden's procedure can be used as before (Section 4.1.2) to obtain the solution of the model equations.

4.2.3 Flash Calculations:

The model developed in section 4.2.1 and the method of solution presented in section 4.2.2 assume that the vapor and liquid flow rates, temperature and compositions of feed stream are known. However, these properties are seldom measured since, before entering the fractionator, the crude oil is heated in a furnace and is allowed to flash on the feed plate. The total mass flow rate of oil, its temperature and pressure at the outlet of the furnace are the only quantities which are known. During its course through the heating furnace the pipeline carrying crude oil receives heat which partially vaporizes the oil. This mixture flashes on entry into the feed plate and in order to find the temperature of feed and individual phase flow rates, flash calculations are performed according to following procedure.

The temperature and pressure of the feed coming out of the furnace at point 1 (figure 6) is specified. Feed mixture in the pipeline will have both phases present at pressure of P_1 and temperature T_1 . The fraction and compositions of the

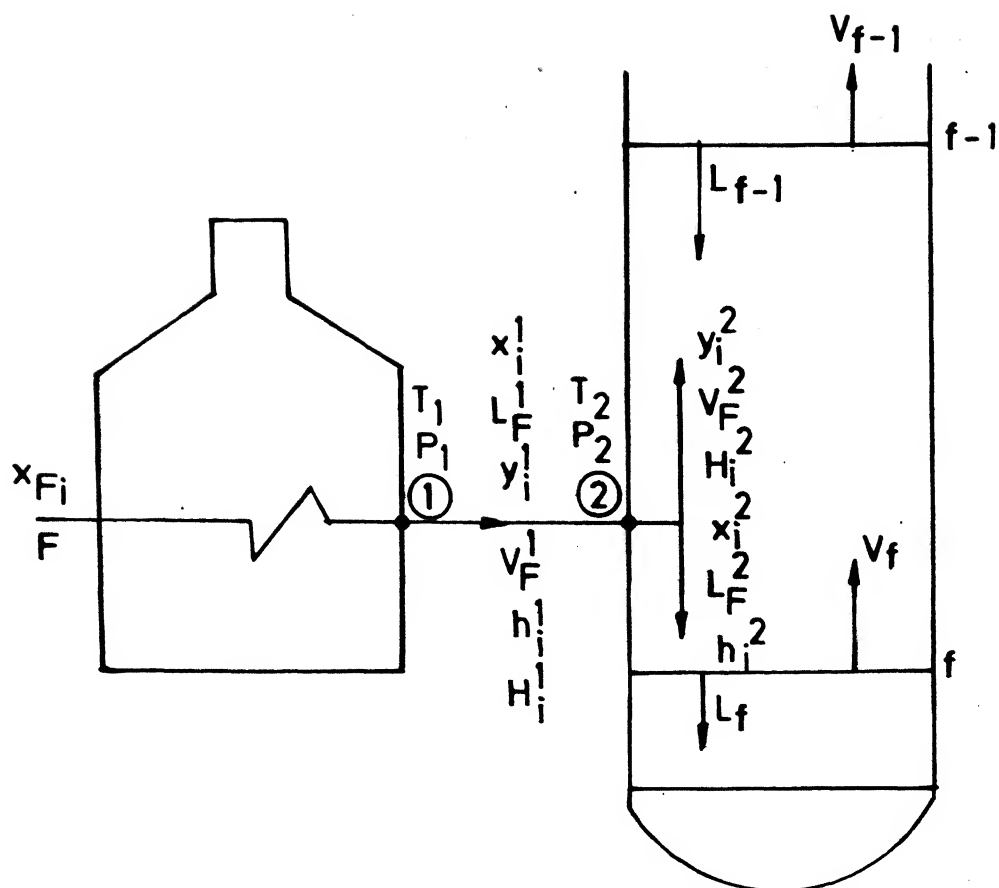


FIG. 6 FEED PLATE FLASH ZONE

components in both phases in the pipeline can be evaluated by isothermal flash calculation as described below. When the temperature and pressure of the flashing zone is specified, the flash is termed as isothermal flash. The material balance and equilibrium relations of this flash calculation is given below:

$$F x_{F_i} = L_F^1 x_i^1 + V_F^1 y_i^1 \quad (4.14)$$

where F = total molar feed rate

x_{F_i} = mole fraction of components in feed

L_F = liquid portion of the feed in the pipe line

V_F = vapor portion of the feed in the pipe line

x_i = mole fraction in liquid

y_i = mole fraction in vapor.

1 refers to the position as shown in the figure.

$$y_i^1 = K_i^1 x_i^1 \quad (4.15)$$

K_i = distribution coefficient

$$\sum_{i=1}^M y_i^1 - \sum_{i=1}^M x_i^1 = 0 \quad (4.16)$$

Equations 4.14, 4.15 and 4.16 can be combined to give

$$\sum_{i=1}^M \frac{x_{F_i} (1 - K_i^1)}{\frac{V_F^1}{F} K_i^1 + (1 - \frac{V_F^1}{F})} = 0 \quad (4.17)$$

The equation 4.17 is solved for $\frac{V_F^1}{F}$ using Newton's method.

If $\frac{V_F^1}{F}$ is found, x_i^1 and y_i^1 can be solved by using the following

equation which is obtained by combining equation 4.14 and 4.15.

$$x_i^1 = \frac{x_{Fi}}{\frac{V_F^1}{F} K_i^1 + (1 - \frac{V_F^1}{F})} \quad (4.18)$$

substituting this value of x_i^1 in equation (4.15) y_i^1 is obtained. Having known the liquid and vapor fraction of feed and their compositions at point 1, the enthalpies at both phases can be calculated at this point. Since, no heat is supplied from external agencies between point 1 and 2 the following heat balance equation holds good.

$$L_F^1 h_F^1 + V_F^1 H_F^1 = L_F^2 h_F^2 + V_F^2 H_F^2 \quad (4.19)$$

where h_F = liquid phase enthalpy

H_F = vapor phase enthalpy

Superscripts 1 and 2 stand for locations 1 and 2 in Figure 6. Now L_F^2 and V_F^2 can be found in the following way. A temperature T_2 is assumed and at that temperature performing isothermal flash calculation as described above V_F^2 and L_F^2 is computed. Then it is checked whether equation (4.19) is satisfied. If not, then a new temperature is calculated using Newton's method, and the calculations are repeated until the convergence is achieved.

4.3 Thermodynamics:

Thermodynamic properties are required to be evaluated for each component at different temperatures and pressures during the distillation calculations. For crude oil distillation also, it is needed to evaluate these properties for the pseudocomponents which represent the composition in present case.

4.3.1 Correlations for Molecular Properties:

Molecular weight, critical temperature and pressure and acentricity factor of each pseudo-component are determined from the correlations given by Lee and Kesler (1975, 1976).

Correlations are as follows:

$$\begin{aligned} MW = & -12272.6 + 9486.4 \text{ SG} + (4.6523 - 3.3287 \text{ SG}) T_b \\ & + (1 - 0.77084 \text{ SG} - 0.02058 \text{ SG}^2) \times (1.3437 - 720.79/T_b) \\ & 10^7/T_b + (1 - 0.80882 \text{ SG} + 0.02226 \text{ SG}^2) \times (1.8828 - \\ & 181.98/T_b) 10^{12}/T_b^3 \end{aligned} \quad (4.20)$$

where MW = molecular weight

SG = specific gravity, 60°F/60°F

T_b = average boiling point, °R (Mean)

$$\begin{aligned} T_c = & 341.7 + 811 \text{ SG} + (0.4244 + 0.1174 \text{ SG}) T_b \\ & + (0.4669 - 3.2623 \text{ SG}) 10^5/T_b \end{aligned} \quad (4.21)$$

where T_c = critical temperature, °R

$$\begin{aligned} \ln P_c = & 8.3634 - 0.0566/\text{SG} - (0.24244 + 2.2898/\text{SG} + 0.11857/\text{SG}^2) 10^{-3} T_b \\ & + (1.4685 + 3.648/\text{SG} + 0.47227/\text{SG}^2) 10^{-7} T_b^2 - (0.42019 + \\ & 1.6977/\text{SG}^2) 10^{-10} T_b^3 \end{aligned} \quad (4.22)$$

where P_c = critical pressure, psi

$$w = -7.904 + 0.1352 K - 0.007465 K^2 + 8.359 T_{br} \\ + (1.408 - 0.01063 K)/T_{br} \quad (4.23)$$

$$\text{for } T_{br} > 0.8$$

$$w = (\ln P_{br}^S - 5.92714 + 6.09648/T_{br} + 1.28862 \ln T_{br} \\ - 0.169347 T_{br}^6)/(15.2518 - 15.6875/T_{br} - 13.4721 \ln T_{br} \\ + 0.43577 T_{br}^6) \quad (4.24)$$

$$\text{for } T_{br} \leq 0.8$$

where w = acentric ~~factor~~ factor

K = Watson characterization factor

$$= T_b^{1/3}/SG$$

T_{br} = Reduced boiling point

P_{br}^S = Reduced vapor pressure

4.3.2 Vapor Liquid Equilibria:

Distribution coefficients or K -values were calculated assuming the system to be ideal, for which the following relation holds good.

$$K_i = P_i^S/P \quad (4.25)$$

where K_i = distribution coefficient of component i

P_i^S = vapor pressure of component i

P = total pressure.

The vapor pressure data required for determination of K -values are based on Maxwell-Bonnell charts in API Technical Data Book (1977). The following equation has been obtained by curve fitting and has been used in the present work.

following relationship:

$$\Delta T = T_b - T_b^1 = 2.5f (K-12) \log \frac{P^S}{14.7} \quad (4.27)$$

where f = corrector factor.

For normal boiling points less than 200°F (i.e. $T_b < 200^\circ\text{F}$) $f=0$. For all subatmospheric ^{vapor pressures} and for all substances having normal boiling points greater than 400°F (i.e. $T_b > 400^\circ\text{F}$) and $(P^S/14.7) < 1.0$ $f=1$. For superatmospheric vapor pressures of substances having normal boiling points between 200°F and 400°F (i.e. $(P^S/14.7) > 1.0$ and $200^\circ\text{F} < T_b < 400^\circ\text{F}$), f is given approximately by the expression

$$f = \frac{T_b - 659.7}{200} \quad (4.28)$$

The ΔT is then subtracted from the true normal boiling point, T_b , to get a new corrected normal boiling point T_b^1 . Now this new value of T_b^1 is used in a new calculation of P^S and the whole calculation procedure is repeated iteratively until the difference between two successive values of the vapor pressure agrees with the desired tolerance.

4.3.3 Enthalpy:

Enthalpy of each pseudocomponent was computed from Lee and Kesler Modification (Lee and Kesler: 1975, 1976; API Data Book: 1977) of John-Greyson (1961) charts for evaluation of enthalpy.

Liquid phase enthalpy for a particular petroleum fraction is given by the following relation:

$$h = A_1(T-259.7) + A_2(T^2-259.7^2) + A_3(T^3 - 259.7^3) \quad (4.29)$$

where h = enthalpy of liquid petroleum fraction, Btu/lb

$$A_1 = 10^{-9} \left[-1171.26 + (23.722 + 24.907 \text{ SG}) + \frac{(1149.82-46.535K)}{\text{SG}} \right]$$

$$A_2 = 10^{-6} \left[(1.0 + 0.82463K) (56.086 - \frac{13.817}{\text{SG}}) \right]$$

$$A_3 = -10^{-9} \left[(1.0 + 0.82463 K) (9.6757 - \frac{2.3653}{\text{SG}}) \right]$$

Vapor phase enthalpy for a petroleum fraction is obtained from the following relation:

$$H = h^* + B_1(T-0.8T_C) + B_2(T^2-0.64 T_C^2) + B_3(T^3-0.512 T_C^3) + \frac{RT_C}{\text{MW}} \left[4.507 + 5.266 w - \left(\frac{\tilde{H}^O}{RT_C} - \tilde{H} \right) \right] \quad (4.30)$$

where H = enthalpy of vapor, Btu/lb

h^* = liquid enthalpy at a reduced temperature of 0.8
calculated by eq.(4.29)

$$B_1 = 10^{-3} \left[-356.44 + 29.72K + B_4(295.02 - \frac{248.46}{\text{SG}}) \right]$$

$$B_2 = 10^{-6} \left[-146.24 + (77.62 - 2.772K)K - B_4(301.42 - \frac{253.87}{\text{SG}}) \right]$$

$$B_3 = 10^{-9} \left[-56.487 - 2.95 B_4 \right]$$

$$B_4 = \left[\left(\frac{12.8}{K} - 1.0 \right) \left(1.0 - \frac{10.0}{K} \right) (\text{SG} - 0.885) (\text{SG}-0.7)(10^4) \right]^2$$

for $10.0 < K < 12.8$ and $0.70 < \text{SG} < 0.885$

= 0 for all other values of K and SG

R = universal gas constant, 1.986 Btu/(lb.mole)(°R)

$\left(\frac{\tilde{H}^O}{RT_C} - \tilde{H} \right)$ = dimensionless pressure effect on enthalpy which can be found by using the following procedure.

$$\left(\frac{\tilde{H}^O - \tilde{H}}{RT_C}\right) = \left(\frac{\tilde{H}^O - \tilde{H}}{RT_{C,o}}\right)^{(o)} + \frac{w}{w^{(h)}} \left[\left(\frac{\tilde{H}^O - \tilde{H}}{RT_{C,h}}\right)^{(h)} - \left(\frac{\tilde{H}^O - \tilde{H}}{RT_{C,o}}\right)^{(o)} \right] \quad (4.31)$$

where $\left(\frac{\tilde{H}^O - \tilde{H}}{RT_{C,o}}\right)^{(o)}$ = effect of pressure on enthalpy for the simple fluid.

$\left(\frac{\tilde{H}^O - \tilde{H}}{RT_{C,h}}\right)^{(h)}$ = effect of pressure on enthalpy for the heavy reference fluid.

T_C = critical temperature of the fluid for which enthalpy is desired, °R

w = acentricity factor of the fluid for which the pressure effect is sought

$w^{(h)}$ = acentricity factor of the heavy reference fluid
= 0.3978.

The dimensionless effects of pressure on the enthalpies of the simple and heavy reference fluid are to be calculated from the following equation:

$$\left(\frac{\tilde{H}^O - \tilde{H}}{RT_{C,i}}\right)^i = -T_r \left\{ Z^{(i)} - 1 - \frac{b_2 + 2b_3/T_r + 3b_4/T_r^2}{T_r V_r} - \frac{C_2 - 3C_3/T_r^2}{2 T_r V_r^2} + \frac{d_2}{5 T_r V_r^5} + 3E \right\} \quad (4.32)$$

where

$$E = \frac{C_4}{2 T_r^3 \gamma} \left\{ \beta + 1 - \left(\beta + 1 + \frac{\gamma}{V_r^2} \right) \exp \left(- \frac{\gamma}{V_r^2} \right) \right\}$$

The superscript i refers to o for simple fluid and to h for the heavy reference fluid.

T_r = reduced temperature, T/T_C

V_r = $P_C V / RT_C$

z^i = compressibility factor of simple fluid ($z^{(o)}$) or heavy reference fluid ($z^{(h)}$).

$b_2, b_3, b_4, c_2, c_3, c_4, d_2, \gamma$ and β are two sets of constants, one set for simple fluid and other for heavy reference fluid given by Lee and Kesler.

In the present work, pressure effect on enthalpy has been neglected in the first approximation.

4.4 User's Mannual:

A computer program has been written in FORTRAN-10 and executed on DEC 1090 system based on the model described earlier. The whole program is divided and kept in six files namely MA FOR, FPREP FOR, XO1.FOR, PR.FOR, GEN2.FOR, FUN1.FOR. The main program and all the subroutines used are discussed below. For details of the program and its usage the program listing given in Appendix B must be referred.

File: MA.FOR

This file contains only the main executive program. All the necessary inputs have to be supplied in this file either through input data file (FOR20.DAT) or data statements. Initial guesses of the variables are also read through an input data file (FOR40.DAT). On successful convergence, it gives the values of the variables at solution which can be either stored in an output file (OUT.DAT) or can be displayed on the terminal screen. The properties of the pseudo-components

are also printed or displayed. The input variables for this program are as follows:

IPRINT:	Printing control parameter = 1; when printing of input data is needed. Any number other than 1 will skip printing these data.
NO	Output control parameter = 05; when results are needed to be displayed on the screen of a terminal = 22; when results are required to be stored in file OUT.DAT.
ITMAX:	Maximum number of iterations permissible.
M:	No. of components
N:	No. of plates
P:	Operating pressure, psia
TBP:	Average boiling point of each pseudo component, °C
API:	API Gravity of each pseudo component
WFR:	Weight fraction of each pseudo component
FEED:	Total mass flow rate of feed, kg/h
TFEED:	Temperature of the feed, °C
PFEED:	Pressure of the feed, psia
NFEED:	Feed plate number
DIS:	Distillate flow rate, kg/h
REFLUX:	Reflux ratio
WL:	Liquid side stream draw off, kgmol/h

WLI & WL2: Flow rates of pumparound reflux streams, kgmol/h
 Q1 & Q2: Heat removal from pumparound reflux streams, Kcal/h
 STM: Rate of steam input to the column/sidestrippers, Kg/h
 File: FPREP.FOR

This file contains subroutines which are needed for feed characterization.

Subroutine FPREP:

This subroutine computes the molecular properties of pseudocomponents and evaluates the vapor and liquid fractions of feed and their composition through flash calculation.

Input data:

FEED, T, P, M, WFR, API, TBP

where T: temperature of feed, °C

P: pressure of feed, psia

Output data: PC, TC, W, AMW, SG, AMWFD, FL, FV, FLC, FVC, ENTHL,
 ENTHV

where PC: Critical pressure of each pseudocomponent, psia

TC: critical temperature of each pseudocomponent, °R

W: acentricity factor

WK: Watson characterization factor

AMW: Molecular weight of each pseudo component

SG: Specific gravity 60°F/60°F

AMWFD: Average molecular weight of feed.

FL: Liquid portion of feed, kgmole/h

FV: Vapor portion of feed, kgmole/h

FLC: Composition of liquid phase of feed, kgmole/h

FVC: Composition of vapor phase of feed, kgmole/h

ENTHL: Enthalpy of liquid phase of feed, kcal/h

ENTHV: Enthalpy of vapor phase of feed, kcal/h

Subroutine FLASH:

This subroutine is used for isothermal flash calculation.

Input Data: FM, XF, T, P, M

where FM: molar flow rate of feed, kgmol/hr

XF: mole fraction of feed

T: temperature at which flash calculation is sought, °C

P: pressure of flash zone, psia

Subroutine EQM1

This subroutine computes ideal K-values using Maxwell-Bonnel vapor pressure correlations.

Input data: T, P, WK, TBP, M

Output data: QK

where QK : K-value of each component

Subroutine FL1

This subroutine performs the adiabatic flash calculation.

Input data: FM, XF, P, M

Output data: ENTHL, ENTHV

File: X01.FOR

File X01.FOR contains all the subroutines necessary to solve component material balance equations.

Subroutine X01

This subroutine generates the coefficient matrix of component material balance equations and then solves calling modified Thomas algorithm subroutine (THOMAS)

Input data: T, N, M, P, REFLUX, RL, V, WL1, WL2, WL, **FLC**, FVC

where T: temperature of each stage, °C

N: total number of stages

RL: liquid flow rate at each stage, kgmol/h

V: vapor flow rate at each stage, kgmol/h

Output data: RLC, RVC

where RLC : component flow rate of liquid at each stage, kgmole/h

RVC: component flow rate of vapor at each stage, kgmole/h

Subroutine THOMAS

Input data: AT, BT, CT, F, OF1, OF2, OF3

where AT, BT, CT: elements of tridiagonal band of the coefficient matrix

OF1, OF2, OF3: Offdiagonal elements in the coefficient matrix

F : right hand side of the component material balance equation

File: GEN2.FOR

This file contains the following subroutines.

Subroutine GENG:

Subroutine GENG computes the discrepancy function of jth plate.

Input data: J, N, NJ, XX, M, REFLUX, FL, FV, ENTLE, ENTVE, WL, WV, STEAM, WL1, WL2, TCOND, RLC, RVC

where J : jth plate

N : total number of equations per stage i.e. 3

NJ : number of stages

XX : vector of independent variables

Output data: G

where G : the vector of discrepancy functions at jth stage.

Subroutine BLOCK

Subroutine BLOCK returns the values of independent variables at solution on successful exit.

Input data: XX, N, NJ, M, P

where NJ: number of stages

N : number of equations per stage

Output data: XX

where XX : the vector of independent variables

Subroutine JAC

This subroutine evaluates the partial derivatives of the Jacobian matrix using numerical differentiation.

Input data: XX, G1, N, M, P

where XX : the values of the independent variables at which
partial derivatives are sought.

G1 : values of the discrepancies at that point

N : number of equations per stage

Output data: PD

where PD: partial derivatives

Subroutine YECMUT

This subroutine performs the multiplication of a matrix
with a vector.

Input data: X, Y, N

where X : matrix

Y : vector

N : order of X matrix

Output data: Z

where Z : resultant vector

File: FUN1.FOR

The file contains only one subroutine.

Subroutine FUN

This subroutine computes the discrepancies of all the
stages.

Input data: XX, N, M, P, WL, WL1, WL2

where N: total number of stages

XX: vector of independent variables

Output data: GT

where GT: the matrix whose elements contains the
discrepancies of all stages.

File: PR.FOR

File PR.FOR contains the all the subroutines required for thermodynamic property estimation i.e. vapor-liquid equilibria and enthalpy.

Subroutine EQIL1:

The subroutine computes K-values (Ideal) using Maxwell-Bonneli correlations for vapor-pressure.

Input data: J, T, P, M, WK, TBP

where J : jth stage

T : temperature of jth stage, °C

P : pressure of jth stage, psia

Output data: RK

where RK : K-values of each component at jth stage.

Subroutine ENTHLP

This subroutine computes the enthalpies of pseudo-components for both phases.

Input data: J, T, P, M, WK, SG

where J : jth stage

T : temperature of jth stage, °C

P : pressure of jth stage, psia

Output data: HL, HV, CPL, CPV

where HL : liquid phase enthalpy of each component at jth stage, kcal/kg mol

HV : vapor phase enthalpy of each component at jth stage, kcal/kg mol.

CPL : specific heat of each component in liquid
phase at jth stage, kcal/kg mol°C

CPV : specific heat of each component in vapor phase
at jth stage, kcal/kg mol°C

Subroutine SHEAT

This subroutine computes enthalpy of steam

Input data: J, T

where J : jth stage

T : temperature of jth stage, °C

Output data: HSTM

where HSTM : enthalpy of steam at jth stage, kcal/kg mol.

CHAPTER 5

RESULTS AND DISCUSSIONS

Using the model developed in the previous chapter, an atmospheric crude oil distillation column has been simulated and the results have been compared with those obtained from a commercial simulation package. Also probable reasons are discussed for the discrepancies observed.

5.1 Statement of the Problem:

The column configuration has been shown in Figure 5. The main column has 13 equilibrium stages (plates) and the three side strippers have 2 plates each. At the bottom, of the main column and each of the side strippers, open steam is introduced at 3.4 atm pressure and 350°C. Steam flow rates are given in the figure. Feed at a rate of 100 tonnes/hr at temperature 340°C and pressure 14 atm is introduced at plate 12. The light ends analysis of the feed is given in Table 5. The TBP and specific gravity data of the crude is given in Table 6. The column is operated at 4 atm pressure. The main column has a total condenser, the temperature of which is 45°C. Distillate flow rate is 160 kgmole/hr. There are two pumparound refluxes employed in the main column. From the 7th tray of the tower a liquid fraction of 616 kgmole/hr is withdrawn and returned to 6th plate after extracting 2.75×10^6 kcal/hr of heat from it. In the second pumparound reflux, a liquid portion of 275 kgmole/hr

is withdrawn from 10th plate and returned to 9th plate after cooling it. The heat removal from this reflux is 2.0×10^6 kcal/hr. A liquid sidestream of 98.43 kgmole/hr is withdrawn from 4th plate and fed to the top plate of first sidestripper and the vapor leaving the top plate of this side stripper is led to 3rd plate in the main column. 178.84 kgmole/hr of liquid withdrawn from the 7th tray of the main column is the feed to the 2nd sidestripper and vapor coming out of this stripper is introduced to plate 6 of the main column. The feed to the last sidestripper is a portion of liquid withdrawn from plate 10. The flow rate of this withdrawn stream is 129.15 kgmole/hr. The stripped vapor from 3rd stripper is sent back to the 9th tray of the main column.

5.2 Results and Discussion:

Molecular properties of the pseudo components as calculated by the correlations of section 4.3 are given in Table 7. In this table the components have been characterized by their average boiling points. The liquid fraction and vapor fraction of the feed and the composition in both phases as computed from flash calculations are tabulated in Table 8. In the same table, the results from the standard solution are also included for comparison. In view of the mismatch, the flash temperature was increased by 9 °C which brought the total vapor and liquid flow rates close to the standard solution. The vapor flow rate was 468.96 (470.15 from standard solution) and the liquid

flow rate was 94.51 (96.04 from standard solution). Two sets of calculations were made, (a) with feed to the column provided from the flash calculation with increased temperature (b) with feed same as that obtained in standard solution.

Table 9 shows a comparison between calculated plate temperatures and total vapor flow rates obtained for the above two cases and the standard solution. As seen from this table deviations from standard solution in case (a) are larger in comparison to case (b). This is to be expected since case (a) represents the added discrepancies of both flash calculations and distillation calculations, whereas case (b) shows only distillation column calculation errors. The possible reasons for these deviations seems to be thermodynamic in nature. The vapor enthalpies calculated in the present program are higher than actual since the pressure correction was not included. This leads to a lower vapor fraction in the flash zone as shown in Table 8. By increasing the temperature of the flash, the vapor fraction is increased to match the standard solution but then, the heat content of vapor will also go up thereby requiring higher reflux. This amounts to higher vapor flow rates through the column as seen in case (a) of table 9. The match between case (b) and the standard solution is more reasonable, all deviations being less than 10 percent. Here again, the enthalpies may be responsible for the observed error. The vapor-liquid equilibrium constants or K-values have been

calculated by application of the idealized Raoult's law where their dependence on composition is not included. This may have also contributed to the loss of accuracy.

Tables 10 and 11 show a comparison of product compositions obtained in present study for cases (a) and (b) with those of standard solution. As expected, the match between case (a) and standard solution is poorer as compared to that between case (b) and the standard.

TABLE 5: LIGHT ENDS ANALYSIS

Component	Weight percent
Propane	0.1
I-Butane	0.1
N-Butane	0.3
I-Pentane	0.3
N-Pentane	0.5

TABLE 6: TBP AND GRAVITY (API) DATA

No.	Cut °C	Cumulative wt.%	API
1	Upto 25	1.9	95.00
2	25 - 50	3.3	85.30
3	50 - 75	7.2	63.60
4	75 - 100	11.9	55.98
5	100 - 125	17.4	52.08
6	125 - 150	22.6	48.02
7	150 - 175	29.1	47.28
8	175 - 200	33.1	45.60
9	200 - 225	36.8	41.76
10	225 - 250	41.4	39.12
11	250 - 275	47.4	34.70
12	275 - 300	51.8	33.22
13	300 - 325	56.8	36.22
14	325 - 350	61.6	33.58
15	350 - 370	65.4	32.42

TABLE 7: MOLECULAR PROPERTIES OF THE PSEUDO-COMPONENTS

No.	Components	wt fraction	SG	K	MW	P _C , psia	T _C , °R	w
1	Propane	0.0016	0.507	14.7	2.15	495.99	669.50	0.0765
2	I-Butane	0.0015	0.563	13.8	60.83	495.92	738.44	0.1465
3	N-Butane	0.0043	0.584	13.5	60.76	495.30	764.93	0.1693
4	I-Pentane	0.0040	0.624	13.1	69.87	473.56	828.45	0.2179
5	N-Pentane	0.0065	0.631	13.0	74.01	460.45	845.54	0.2313
6	43 C	0.0254	0.643	12.9	76.32	463.05	859.60	0.2408
7	56	0.0251	0.668	12.6	82.57	463.30	892.69	0.2621
8	69	0.0256	0.718	11.9	85.91	505.02	933.05	0.2715
9	83	0.0295	0.734	11.8	93.14	490.48	963.91	0.2902
10	97	0.0303	0.752	11.6	99.70	485.09	997.05	0.3058
11	111	0.0332	0.761	11.6	108.05	457.58	1022.92	0.3307
12	125	0.0320	0.770	11.6	116.04	436.82	1050.06	0.3541
13	139	0.0307	0.779	11.6	124.17	417.53	1076.84	0.3782
14	153	0.0358	0.787	11.6	132.61	398.29	1102.81	0.4036
15	166	0.0379	0.789	11.7	141.29	375.27	1124.08	0.4319
16	180	0.0244	0.792	11.8	150.90	352.62	1146.78	0.4630
17	198	0.0230	0.794	11.9	160.98	330.61	1168.55	0.4958

Table 7 contd.

No.	Components	wt fraction	SG	K	MW	P _C ,psia	T _C °R	W
18	208	0.0212	0.804	11.9	170.40	318.66	1194.39	0.5223
19	222	0.0225	0.814	11.8	180.18	307.47	1219.99	0.5490
20	236	0.0258	0.821	11.8	190.74	294.15	1243.90	0.5787
21	250	0.0296	0.828	11.8	201.79	281.14	1267.36	0.6093
22	264	0.0329	0.840	11.8	212.36	274.21	1293.90	0.6340
23	278	0.0262	0.851	11.7	223.52	266.26	1319.49	0.6602
24	291	0.0236	0.855	11.8	235.25	253.87	1339.57	0.6921
25	305	0.0267	0.854	11.9	249.33	236.64	1357.69	0.7340
26	319	0.0273	0.840	12.2	266.46	210.00	1367.51	0.7938
27	333	0.0261	0.847	12.2	280.17	201.37	1389.93	0.8277
28	347	0.0257	0.855	12.1	293.97	194.20	1413.10	0.8600
29	361	0.0254	0.859	12.2	309.04	184.41	1433.55	0.8984
30	375	0.0243	0.865	12.2	324.02	176.59	1455.21	0.9339
31	396	0.0477	0.876	12.1	346.49	167.08	1489.02	0.9813
32	423	0.0469	0.891	12.1	375.98	155.24	1532.73	1.0395
33	451	0.0460	0.907	12.0	407.00	146.35	1578.34	1.0963

Table 7 contd.

No.	Components	wt fraction	SG	K	MW	P _C , psia	T _C °R	W
34	479	0.0452	0.924	12.0	437.87	138.02	1624.74	1.1488
35	507	0.0444	0.941	11.9	468.96	130.06	1670.58	1.1999
36	535	0.0436	0.958	11.8	499.46	123.06	1717.09	1.2474
37	554	0.0181	0.971	11.8	519.00	119.36	1749.97	1.2757

Note: Properties of pure components (Propane - n-Pentane) should preferably be taken from standard sources.

TABLE 8: COMPARISON OF FEED COMPOSITION IN BOTH PHASES OBTAINED FROM FLASH CALCULATION
WITH STANDARD SOLUTION

Component	Composition in liquid, kg mole/h		Composition in vapour, kgmole/h	
	Present Method	Standard	Present method	Standard
1	0.3591 x 10 ⁻²	0.2915 x 10 ⁻¹	0.1943 x 10 ¹	0.3679 x 10 ¹
2	0.6946 x 10 ⁻²	0.2846 x 10 ⁻¹	0.2458 x 10 ¹	0.2507 x 10 ¹
3	0.2389 x 10 ⁻¹	0.8459 x 10 ⁻¹	0.7053 x 10 ¹	0.7247 x 10 ¹
4	0.2813 x 10 ⁻¹	0.8591 x 10 ⁻¹	0.5695 x 10 ¹	0.5438 x 10 ¹
5	0.4843 x 10 ⁻¹	0.1455	0.8734 x 10 ¹	0.8965 x 10 ¹
6	0.1991	0.5200	0.3307 x 10 ²	0.3055 x 10 ²
7	0.2215	0.5497	0.3017 x 10 ²	0.2851 x 10 ²
8	0.2509	0.5947	0.2953 x 10 ²	0.2847 x 10 ²
9	0.3383	0.7150	0.3133 x 10 ²	0.3078 x 10 ²
10	0.3967	0.7675	0.2999 x 10 ²	0.2987 x 10 ²
11	0.4912	0.8829	0.3032 x 10 ²	0.3058 x 10 ²
12	0.5405	0.8910	0.2703 x 10 ²	0.2743 x 10 ²
13	0.5951	0.9015	0.2412 x 10 ²	0.2466 x 10 ²
14	0.7990	0.1112 x 10 ¹	0.2619 x 10 ²	0.2692 x 10 ²
15	0.9616	0.1249 x 10 ¹	0.2586 x 10 ²	0.3638 x 10 ²
16	0.7135	0.8629 x	0.1545 x 10 ²	0.1575 x 10 ²
17	0.7767	0.8822	0.1351 x 10 ²	0.1374 x 10 ²
18	0.8364	0.8918	0.1160 x 10 ²	0.1184 x 10 ²
19	0.1038 x 10 ¹	0.1051 x 10 ¹	0.1144 x 10 ²	0.1177 x 10 ²

Table 8 contd.

1	2	3	4	5
20	0.1391 x 10 ¹	0.1341 x 10 ¹	0.1213 x 10 ²	0.1249 x 10 ²
21	0.1865 x 10 ¹	0.1730 x 10 ¹	0.1280 x 10 ²	0.1327 x 10 ²
22	0.2434 x 10 ¹	0.2173 x 10 ¹	0.1305 x 10 ²	0.1367 x 10 ²
23	0.2268 x 10 ¹	0.1966 x 10 ¹	0.9453 x 10 ¹	0.1005 x 10 ²
24	0.2342 x 10 ¹	0.2009 x 10 ¹	0.7689 x 10 ¹	0.8239 x 10 ¹
25	0.3040 x 10 ¹	0.2541 x 10 ¹	0.7667 x 10 ¹	0.8290 x 10 ¹
26	0.3504 x 10 ¹	0.2832 x 10 ¹	0.6740 x 10 ¹	0.7345 x 10 ¹
27	0.3800 x 10 ¹	0.3030 x 10 ¹	0.5515 x 10 ¹	0.6219 x 10 ¹
28	0.4191 x 10 ¹	0.3327 x 10 ¹	0.4550 x 10 ¹	0.5370 x 10 ¹
29	0.4554 x 10 ¹	0.3593 x 10 ¹	0.3664 x 10 ¹	0.4548 x 10 ¹
30	0.4715 x 10 ¹	0.3719 x 10 ¹	0.2783 x 10 ¹	0.3667 x 10 ¹
31	0.1009 x 10 ²	0.8109 x 10 ¹	0.3674 x 10 ¹	0.5420 x 10 ¹
32	0.1049 x 10 ²	0.8768 x 10 ¹	0.1980 x 10 ¹	0.3404 x 10 ¹
33	0.1035 x 10 ²	0.9286 x 10 ¹	0.9440	0.1718 x 10 ¹
34	0.9907 x 10 ¹	0.9141 x 10 ¹	0.4149	0.8568
35	0.9298 x 10 ¹	0.8732 x 10 ¹	0.1695	0.3965
36	0.9465 x 10 ¹	0.8205 x 10 ¹	0.1011	0.1723
37	0.4410 x 10 ¹	0.3286 x 10 ¹	0.9960 x 10 ⁻²	0.3877 x 10 ⁻¹
Total	104.67	96.04	458.79	470.15

TABLE 9: COMPARISON OF TOTAL VAPOR FLOW RATES AND TEMPERATURES WITH STANDARD SOLUTION

Stage	Present Method		Standard Solution	
	Case (a)	Case (b)	Vapor flow rate $\times 10^{-3}$	Temperature $^{\circ}\text{C}$ $\times 10^{-3}$
	Vapor flow Kgmol/hr $\times 10^{-3}$	Vapor flow rate $\times 10^{-3}$		
	Temperature, $^{\circ}\text{C}$ $\times 10^{-3}$	Temperature, $^{\circ}\text{C}$ $\times 10^{-3}$		
1	0.2600	0.2600	0.2600	0.0450
2	1.1091	0.7504	0.7340	0.1227
3	1.1145	0.8439	0.8670	0.1431
4	0.9797	0.7733	0.8150	0.1585
5	0.8699	0.7264	0.7800	0.1736
6	0.7768	0.6727	0.7280	0.1899
7	0.9137	0.8076	0.8840	0.2057
8	0.8203	0.7335	0.8090	0.2385
9	0.7029	0.6383	0.7020	0.2686
10	0.6838	0.6288	0.6950	0.2917
11	0.5766	0.5384	0.5950	0.3359
12	0.0643	0.0665	0.0660	0.3502
13	0.0482	0.0485	0.0500	0.3468
14	0.0352	0.0316	0.0330	0.1479
15	0.0239	0.0218	0.0220	0.1391
16	0.0637	0.0614	0.0660	0.1961
17	0.0429	0.0417	0.0430	0.1878
18	0.0575	0.0558	0.0620	0.2846
19	0.0423	0.0415	0.0440	0.2781

Distillate composition in Kgmoles/hr			Product composition from Stripper 1 in Kgmoles/hr			
Present Method		Standard solution	Present Method		Standard solution	
Case (a)	Case (b)		Case (a)	Case (b)		
2		4	5		6	7
0.3708 x 10 ¹	0.3707 x 10 ¹	0.3705 x 10 ¹	0.4403 x 10 ⁻³	0.7807 x 10 ⁻³	0.1161 x 10 ⁻²	
0.2533 x 10 ¹	0.2532 x 10 ¹	0.2527 x 10 ¹	0.1739 x 10 ⁻²	0.3025 x 10 ⁻²	0.4781 x 10 ⁻²	
0.7318 x 10 ¹	0.7310 x 10 ¹	0.7298 x 10 ¹	0.9592 x 10 ⁻²	0.1649 x 10 ⁻¹	0.1938 x 10 ⁻¹	
0.5476 x 10 ¹	0.5451 x 10 ¹	0.5430 x 10 ¹	0.3478 x 10 ⁻¹	0.5759 x 10 ⁻¹	0.6136 x 10 ⁻¹	
0.8992 x 10 ¹	0.8928 x 10 ¹	0.8921 x 10 ¹	0.9020 x 10 ⁻¹	0.1475	0.1304	
0.3031 x 10 ²	0.3001 x 10 ²	0.3005 x 10 ²	0.4213	0.6834	0.57508	
0.2792 x 10 ²	0.2735 x 10 ²	0.2752 x 10 ²	0.8700	0.1382 x 10 ¹	0.1136 x 10 ¹	
0.2672 x 10 ²	0.2561 x 10 ²	0.2576 x 10 ²	0.1382 x 10 ¹	0.2839 x 10 ¹	0.2577 x 10 ¹	
0.2597 x 10 ²	0.2365 x 10 ²	0.2451 x 10 ²	0.4402 x 10 ¹	0.6502 x 10 ¹	0.5591 x 10 ¹	
0.1953 x 10 ²	0.1610 x 10 ²	0.1806 x 10 ²	0.8717 x 10 ¹	0.1174 x 10 ²	0.1000 x 10 ²	
0.1149 x 10 ²	0.8279 x 10 ¹	0.1079 x 10 ²	0.1431 x 10 ²	0.1702 x 10 ²	0.1538 x 10 ²	
0.3859 x 10 ¹	0.2505 x 10 ¹	0.3975 x 10 ¹	0.1404 x 10 ²	0.1523 x 10 ²	0.1535 x 10 ²	
0.8582 x	0.5359	0.1043 x 10 ¹	0.9485 x 10 ¹	0.1003 x 10 ²	0.1135 x 10 ²	
0.1712	0.1067	0.25274	0.5958 x 10 ¹	0.6379 x 10 ¹	0.8024 x 10 ¹	
0.2898 x 10 ⁻¹	0.1813 x 10 ⁻¹	0.4499 x 10 ⁻¹	0.3027 x 10 ¹	0.3307 x 10 ¹	0.4310 x 10 ¹	
0.2279 x 10 ⁻²	0.1431 x 10 ⁻²	0.4309 x 10 ⁻²	0.8093	0.9048	0.1270 x 10 ¹	
0.2319 x 10 ⁻³	0.1465 x 10 ⁻³	0.5544 x 10 ⁻³	0.2926	0.3361	0.5111	
0.2061 x 10 ⁻⁴	0.1328 x 10 ⁻⁴	0.6487 x 10 ⁻⁴	0.9572 x 10 ⁻¹	0.1145	0.1896	
0.1816 x 10 ⁻⁵	0.1222 x 10 ⁻⁵	0.8005 x 10 ⁻⁵	0.8194 x 10 ⁻¹	0.4078 x 10 ⁻¹	0.7517 x 10 ⁻¹	
0.1368 x 10 ⁻⁶	0.9831 x 10 ⁻⁷	0.9394 x 10 ⁻⁶	0.9636 x 10 ⁻²	0.1344 x 10 ⁻¹	0.2874 x 10 ⁻¹	
0.8296 x 10 ⁻⁸	0.6406 x 10 ⁻⁸	0.9599 x 10 ⁻⁷	0.2450 x 10 ⁻²	0.3764 x 10 ⁻²	0.9681 x 10 ⁻²	
0.4032 x 10 ⁻⁹	0.3302 x 10 ⁻⁹	0.8256 x 10 ⁻⁸	0.5237 x 10 ⁻³	0.8748 x 10 ⁻³	0.2764 x 10 ⁻²	

TABLE 10: COMPARISON OF RESULTS OF PRESENT MODEL WITH STANDARD SOLUTION

Component	Distillate composition in Kgmoles/hr				Product composition from Stripper 1 in Kgmoles/hr			
	Present Method		Standard solution		Present Method		Standard solution	
	Case (a)	Case (b)			Case (a)	Case (b)		
1	0.3708 x 10 ⁻¹	0.3707 x 10 ⁻¹	0.3705 x 10 ⁻¹	1	0.4403 x 10 ⁻³	0.7807 x 10 ⁻³	0.1161 x 10 ⁻²	2
2	0.2533 x 10 ⁻¹	0.2532 x 10 ⁻¹	0.2527 x 10 ⁻¹	1	0.1739 x 10 ⁻²	0.3025 x 10 ⁻²	0.4781 x 10 ⁻²	2
3	0.7318 x 10 ⁻¹	0.7310 x 10 ⁻¹	0.7298 x 10 ⁻¹	1	0.9592 x 10 ⁻²	0.1649 x 10 ⁻¹	0.1938 x 10 ⁻¹	1
4	0.5476 x 10 ⁻¹	0.5451 x 10 ⁻¹	0.5430 x 10 ⁻¹	1	0.3478 x 10 ⁻¹	0.5759 x 10 ⁻¹	0.6136 x 10 ⁻¹	1
5	0.8992 x 10 ⁻¹	0.8928 x 10 ⁻¹	0.8921 x 10 ⁻¹	1	0.9020 x 10 ⁻¹	0.1475	0.1304	
6	0.3031 x 10 ⁻²	0.3001 x 10 ⁻²	0.3005 x 10 ⁻²	2	0.4213	0.6834	0.57508	
7	0.2792 x 10 ⁻²	0.2735 x 10 ⁻²	0.2752 x 10 ⁻²	2	0.8700	0.1382 x 10 ⁻¹	0.1136 x 10 ⁻¹	1
8	0.2672 x 10 ⁻²	0.2561 x 10 ⁻²	0.2576 x 10 ⁻²	2	0.1382 x 10 ⁻¹	0.2839 x 10 ⁻¹	0.2577 x 10 ⁻¹	1
9	0.2597 x 10 ⁻²	0.2365 x 10 ⁻²	0.2451 x 10 ⁻²	2	0.4402 x 10 ⁻¹	0.6502 x 10 ⁻¹	0.5591 x 10 ⁻¹	1
10	0.1953 x 10 ⁻²	0.1610 x 10 ⁻²	0.1806 x 10 ⁻²	2	0.8717 x 10 ⁻¹	0.1174 x 10 ⁻²	0.1000 x 10 ⁻²	2
11	0.1149 x 10 ⁻²	0.8279 x 10 ⁻¹	0.1079 x 10 ⁻²	1	0.1431 x 10 ⁻²	0.1702 x 10 ⁻²	0.1538 x 10 ⁻²	2
12	0.3859 x 10 ⁻¹	0.2505 x 10 ⁻¹	0.3975 x 10 ⁻¹	1	0.1404 x 10 ⁻²	0.1523 x 10 ⁻²	0.1535 x 10 ⁻²	2
13	0.8582 x	0.5359	0.1043 x 10 ⁻¹	1	0.9485 x 10 ⁻¹	0.1003 x 10 ⁻²	0.1135 x 10 ⁻²	2
14	0.1712	0.1067	0.25274		0.5958 x 10 ⁻¹	0.6379 x 10 ⁻¹	0.8024 x 10 ⁻¹	1
15	0.2898 x 10 ⁻¹	0.1813 x 10 ⁻¹	0.4499 x 10 ⁻¹	1	0.3027 x 10 ⁻¹	0.3307 x 10 ⁻¹	0.4310 x 10 ⁻¹	1
16	0.2279 x 10 ⁻²	0.1431 x 10 ⁻²	0.4309 x 10 ⁻²	2	0.8093	0.9048	0.1270 x 10 ⁻¹	1
17	0.2319 x 10 ⁻³	0.1465 x 10 ⁻³	0.5544 x 10 ⁻³	3	0.2926	0.3361	0.5111	
18	0.2061 x 10 ⁻⁴	0.1328 x 10 ⁻⁴	0.6487 x 10 ⁻⁴	4	0.9572 x 10 ⁻¹	0.1145	0.1896	
19	0.1816 x 10 ⁻⁵	0.1222 x 10 ⁻⁵	0.8005 x 10 ⁻⁵	5	0.8194 x 10 ⁻¹	0.4078 x 10 ⁻¹	0.7517 x 10 ⁻¹	1
20	0.1368 x 10 ⁻⁶	0.9831 x 10 ⁻⁷	0.9394 x 10 ⁻⁶	7	0.9636 x 10 ⁻²	0.1344 x 10 ⁻¹	0.2874 x 10 ⁻¹	1
21	0.8296 x 10 ⁻⁸	0.6406 x 10 ⁻⁸	0.9599 x 10 ⁻⁷	8	0.2450 x 10 ⁻²	0.3764 x 10 ⁻²	0.9681 x 10 ⁻²	2
22	0.4032 x 10 ⁻⁹	0.3302 x 10 ⁻⁹	0.8256 x 10 ⁻⁸	9	0.5237 x 10 ⁻³	0.8748 x 10 ⁻³	0.2764 x 10 ⁻²	2

Table 10 contd.

1	2	3	4	5	6	7
23	0.1257×10^{-10}	0.1071×10^{-10}	0.4568×10^{-9}	0.7320×10^{-4}	0.1302×10^{-3}	0.5131×10^{-3}
24	0.4539×10^{-12}	0.3937×10^{-12}	0.2631×10^{-10}	0.1177×10^{-4}	0.2183×10^{-4}	0.1009×10^{-3}
25	0.1407×10^{-13}	0.1230×10^{-13}	0.1822×10^{-11}	0.1925×10^{-5}	0.3713×10^{-5}	0.2407×10^{-4}
26	0.2966×10^{-15}	0.2584×10^{-15}	0.1301×10^{-12}	0.2485×10^{-6}	0.4937×10^{-6}	0.5631×10^{-5}
27.	0.6401×10^{-17}	0.5582×10^{-17}	0.7054×10^{-14}	0.3076×10^{-7}	0.6233×10^{-7}	0.1063×10^{-5}
28	0.1376×10^{-18}	0.1205×10^{-18}	0.3722×10^{-15}	0.3776×10^{-8}	0.7943×10^{-8}	0.2014×10^{-6}
29	0.2154×10^{-20}	0.1887×10^{-20}	0.1983×10^{-16}	0.3964×10^{-9}	0.8594×10^{-9}	0.3809×10^{-7}
30	0.3094×10^{-22}	0.2730×10^{-22}	0.9159×10^{-18}	0.3793×10^{-10}	0.8502×10^{-10}	0.0000
31	0.9687×10^{-25}	0.8716×10^{-25}	0.1608×10^{-19}	0.2059×10^{-11}	0.4876×10^{-11}	0.0000
32	0.1217×10^{-28}	0.1125×10^{-28}	0.1980×10^{-22}	0.1283×10^{-13}	0.3269×10^{-13}	0.0000
33	0.6420×10^{-33}	0.6101×10^{-33}	0.0000	0.4068×10^{-16}	0.1110×10^{-15}	0.0000
34	0.1686×10^{-37}	0.1608×10^{-37}	0.0000	0.8158×10^{-19}	0.2327×10^{-18}	0.0000
35	0.0000	0.0000	0.0000	0.1222×10^{-21}	0.3577×10^{-21}	0.0000
36	0.0000	0.0000	0.0000	0.1313×10^{-24}	0.3904×10^{-24}	0.0000
37	0.0000	0.0000	0.0000	0.3953×10^{-27}	0.1176×10^{-26}	0.0000

TABLE 11: COMPARISON OF RESULTS OF PRESENT MODEL WITH STANDARD SOLUTION

Component	Production composition from Stripper 2				Product composition from Stripper 3			
	Present Method		Standard solution		Present Method		Standard solution	
	Case (a)	Case (b)			Case (a)	Case (b)		
1	0.1944×10^{-3}	0.2424×10^{-3}	0.7788×10^{-3}	10^{-3}	0.1021×10^{-4}	0.1149×10^{-4}	0.1838×10^{-3}	10^{-3}
2	0.6832×10^{-3}	0.8498×10^{-3}	0.2752×10^{-2}	10^{-2}	0.2886×10^{-4}	0.3228×10^{-4}	0.4666×10^{-3}	10^{-3}
3	0.3627×10^{-2}	0.4504×10^{-2}	0.1043×10^{-1}	10^{-1}	0.1420×10^{-3}	0.1586×10^{-3}	0.1588×10^{-2}	10^{-2}
4	0.1197×10^{-1}	0.1477×10^{-1}	0.2657×10^{-1}	10^{-1}	0.8991×10^{-3}	0.4429×10^{-3}	0.3387×10^{-2}	10^{-2}
5	0.3000×10^{-1}	0.3693×10^{-1}	0.5133×10^{-1}	10^{-1}	0.9528×10^{-3}	0.1056×10^{-2}	0.6247×10^{-2}	10^{-2}
6	0.1362	0.1673	0.2065		0.4265×10^{-2}	0.4716×10^{-2}	0.2477×10^{-1}	10^{-1}
7	0.2576	0.3146	0.3449		0.7559×10^{-2}	0.8436×10^{-2}	0.3556×10^{-1}	10^{-1}
8	0.4906	0.5955	0.6552		0.1391×10^{-1}	0.1526×10^{-1}	0.5097×10^{-1}	10^{-1}
9	0.1088×10^1	0.1309×10^1	0.1281×10^1	10^1	0.2858×10^{-1}	0.3118×10^{-1}	0.7894×10^{-1}	10^{-1}
10	0.2330×10^1	0.2724×10^1	0.2425×10^1	10^1	0.5255×10^{-1}	0.5695×10^{-1}	0.1082	
11	0.5535×10^1	0.6045×10^1	0.5069×10^1	10^1	0.1020	0.1044	0.1635	
12	0.1022×10^2	0.1038×10^2	0.8712×10^1	10^1	0.1738	0.1833	0.2257	
13	0.1488×10^2	0.1467×10^2	0.1277×10^2	10^2	0.2986	0.3064	0.3240	
14	0.2120×10^2	0.2088×10^2	0.1906×10^2	10^2	0.6250	0.6188	0.5857	
15	0.2334×10^2	0.2317×10^2	0.2213×10^2	10^2	0.1117×10^1	0.1064×10^1	0.9852	
16	0.1443×10^2	0.1449×10^2	0.1418×10^2	10^2	0.1269×10^1	0.1156×10^1	0.1022×10^1	10^1
17	0.1210×10^2	0.1237×10^2	0.1237×10^2	10^2	0.2073×10^1	0.1812×10^1	0.1557×10^1	10^1
18	0.9203×10^1	0.9743×10^1	0.1000×10^2	10^2	0.3220×10^1	0.2740×10^1	0.2315×10^1	10^1
19	0.7141×10^1	0.8073×10^1	0.8587×10^1	10^1	0.5300×10^1	0.4522×10^1	0.3818×10^1	10^1
20	0.5060×10^1	0.6218×10^1	0.7040×10^1	10^1	0.8154×10^1	0.7212×10^1	0.6206×10^1	10^1
21	0.3057×10^1	0.4143×10^1	0.5058×10^1	10^1	0.1095×10^2	0.1019×10^2	0.9038×10^1	10^1

Table 11 contd.

1	2	3	4	5	6	7
22	0.1577×10^1	0.2331×10^1	0.3090×10^1	0.1272×10^2	0.1245×10^2	0.1139×10^2
23	0.5366	0.8486	0.1223×10^1	0.9825×10^1	0.9982×10^1	0.9349×10^1
24	0.2054	0.3412	0.5097	0.8131×10^1	0.8482×10^1	0.8048×10^1
25	0.8788×10^{-1}	0.1526	0.2550	0.8051×10^1	0.8595×10^1	0.8195×10^1
26	0.3175×10^{-1}	0.5737×10^{-1}	0.1173	0.6883×10^1	0.7508×10^1	0.7179×10^1
27	0.1083×10^{-1}	0.2029×10^{-1}	0.4762×10^{-1}	0.5518×10^1	0.6156×10^1	0.5920×10^1
28	0.3688×10^{-2}	0.7173×10^{-2}	0.1942×10^{-2}	0.4426×10^1	0.5063×10^1	0.4905×10^1
29	0.1163×10^{-2}	0.2355×10^{-2}	0.7833×10^{-2}	0.3402×10^1	0.4005×10^1	0.3930×10^1
30	0.3373×10^{-3}	0.7128×10^{-3}	0.2943×10^{-2}	0.2425×10^1	0.29504×10^1	0.2951×10^1
31	0.9913×10^{-4}	0.2242×10^{-3}	0.1298×10^{-2}	0.2812×10^1	0.3614×10^1	0.3782×10^1
32	0.6268×10^{-5}	0.1552×10^{-4}	0.1443×10^{-3}	0.1149×10^1	0.1591×10^1	0.1814×10^1
33	0.2356×10^{-6}	0.6359×10^{-6}	0.3780×10^{-5}	0.3255	0.4838	0.5411
34	0.6585×10^{-8}	0.1889×10^{-7}	0.1766×10^{-6}	0.7920×10^1	0.1231	0.1523
35	0.1424×10^{-4}	0.4247×10^{-9}	0.0000	0.1520×10^1	0.2582×10^{-1}	0.3563×10^{-1}
36	0.23911×10^{-11}	0.7309×10^{-11}	0.0000	0.2556×10^{-2}	0.4617×10^{-2}	0.7157×10^{-2}
37	0.5109×10^{-13}	0.1583×10^{-12}	0.0000	0.3336×10^{-3}	0.5394×10^{-3}	0.8895×10^{-3}

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

The mathematical model developed in the present study for multicomponent fractionation has been found to be computationally stable and effective. The model gave results comparable to those reported by Holland for a 11 component problem. This method has been extended to solve crude oil distillation problem using pseudo-component concept and the results have been compared with those obtained with a standard package. The probable reasons for the discrepancies have been discussed. Pressure gradient throughout the column which was neglected for the sake of simplicity may actually influence the results. It is hoped that making necessary corrections to account for effect of pressure on enthalpy and using an appropriate nonideal equation of state for VLE calculation will improve the results.

This work can be extended on following lines to develop a complete simulation package for the crude oil distillation. In the work initial guesses for all independent variables were supplied to solve the problem. But to make the program more effective, an in-built procedure to generate the initial guesses should be developed. This can be done by making use of empirical short cut methods of crude oil distillation calculation such as one discussed by Watkins (1979). Using this method

temperature, vapor and liquid flows at all key trays of the tower can be computed and then by linear interpolation they can give rise to the initial guesses for the independent variables at all stages. In the present work, the liquid streams withdrawn from the main column (kg moles/h) were taken as specification. But in actual practice the products from the side strippers (kg/h) will be the specifications. This can be obtained by modifying the subroutines for calculation of discrepancy functions. Another important specifications in crude oil distillation is amount of overflash. This also should be properly accounted for. Since efficiency, in case of crude oil distillation, is very difficult to define, an analogue column has to be found by trial which contains equilibrium stages but performs like the real column. Since Naphthali-Sandholm method can handle non-ideal thermodynamics, can incorporate efficiencies and is known to have better convergence characteristics, it may be worthwhile to approach the modelling of crude oil distillation using this method on a machine which has sufficient memory.

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APPENDIX A

NAPHTHALI-SANDHOLM FORMULATION OF CRUDE OIL DISTILLATION PROBLEM

For Naphthali-Sandholm method the functions to be solved are component material balance equations for each plate, the equilibrium relationships and enthalpy balance equation for each plate. The material balance and enthalpy balance equations are same as Eqs. 4.12 and 4.11. Only equilibrium relations will be described in this section.

$$Q_{j,i} = \frac{v_{j,i}}{V_j} - \frac{E_{j,i} K_{j,i} l_{j,i}}{L_j} - (1 - E_{j,i}) \frac{v_{j+1,i} + v_{m,i}}{V_{j+1} + V_m} \quad (\text{A.1})$$

for $j = 3, 6, 9$

where m is number of the plate other than $(j+1)$ th plate from which vapor is introduced to the j th plate of the column.

$$Q_{j,i} = \frac{v_{j,i}}{V_j} - K_{j,i} \frac{l_{j,i}}{L_j} \quad ; \quad j = 13, 15, 17, 19 \quad (\text{A.2})$$

$$Q_{j,i} = \frac{v_{j,i}}{V_j} - E_{j,i} K_{j,i} \frac{l_{j,i}}{L_j} - (1 - E_{j,i}) \frac{v_{j+1,i}}{V_{j+1}} \quad (\text{A.3})$$

for all other plates.

Since the last plates of the column (13, 15, 17, 19) do not have any plate below them, it is not possible to define Murphree-plate efficiency for them. That is why the efficiency in this case has been assumed to be unity. In this method dependent variables, total liquid flow rate and vapor flow rates, are calculated by summing up the component flow rates.

Solution technique:

The functions and the variables are grouped stagewise. They are solved simultaneously by N-R technique where

$$\bar{J} \Delta \bar{X}^K = -F(\bar{X}^K)$$

and

$$\bar{X}^{k+1} = \bar{X}^k + \beta \Delta \bar{X}^k$$

The Jacobian matrix has got the same structure as that shown in Table 3. Only difference is that, the elements of matrix shown in Table 3 are algebraic numbers, where as in this case, they will matrix blocks of order $(2M + 1)$. The Jacobian matrix can be solved using modified block Thomas algorithm. The algorithm developed in Section (4.2) to solve the component material balance equations is used. In the developed algorithm as shown, the operations like addition, subtraction, division are algebraic as the elements are algebraic numbers, but in this case there will be matrix operations as the elements of the Jacobian are matrices.

To facilitate the convergence, one damping factor is used which is calculated using Golden Section Search technique.

APPENDIX B

PROGRAM LISTING